



Full wwPDB EM Validation Report ⓘ

Sep 24, 2026 – 05:05 pm BST

PDB ID : 9TKR / pdb_00009tkr
EMDB ID : EMD-56038
Title : E. coli 70S elongation competent complex (70S EC)
Authors : Guerra, G.S.; Demo, G.
Deposited on : 2025-12-10
Resolution : 2.90 Å (reported)
Based on initial model : 6WDD

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

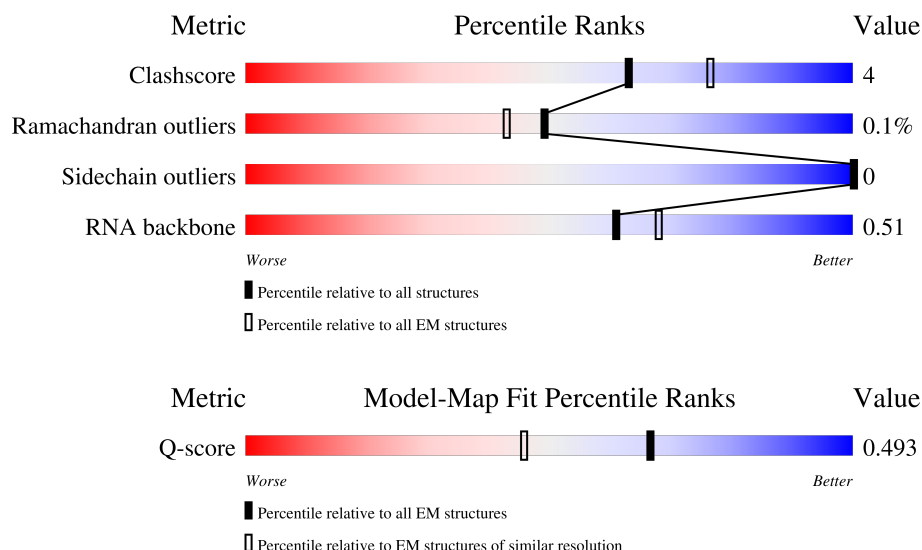
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



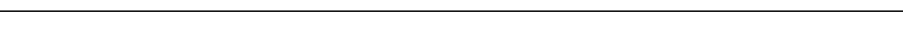
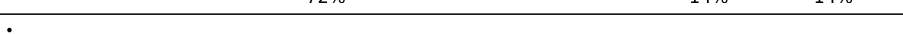
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13054 (2.40 - 3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	241	
2	AB	233	
3	AC	206	

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Mol	Chain	Length	Quality of chain
4	AD	167	
5	AE	135	
6	AF	179	
7	AG	130	
8	AH	130	
9	AI	103	
10	AJ	129	
11	AK	124	
12	AL	118	
13	AM	101	
14	AN	89	
15	AO	82	
16	AP	84	
17	AQ	75	
18	AR	92	
19	AS	87	
20	AT	71	
21	B0	85	
22	B1	78	
23	B2	63	
24	B3	59	
25	B5	57	
26	B6	55	
27	B7	46	
28	B8	65	

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Mol	Chain	Length	Quality of chain
29	B9	38	
30	BA	234	
31	BB	273	
32	BC	209	
33	BD	201	
34	BE	179	
35	BF	177	
36	BI	149	
37	BK	142	
38	BM	142	
39	BN	123	
40	BO	144	
41	BP	136	
42	BQ	127	
43	BR	117	
44	BS	115	
45	BT	118	
46	BU	103	
47	BV	110	
48	BW	100	
49	BX	104	
50	BY	94	
51	D1	1540	
52	D2	2903	
53	D3	120	

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Mol	Chain	Length	Quality of chain
54	D4	56	
55	D5	78	

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 145708 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	225	Total	C	N	O	S	0	0
			1756	1111	315	322	8		

- Molecule 2 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 3 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AC	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 4 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AD	157	Total	C	N	O	S	0	0
			1156	719	218	213	6		

- Molecule 5 is a protein called Small ribosomal subunit protein bS6, fully modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AE	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 6 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AF	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 7 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AG	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 8 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AH	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 9 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AI	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 10 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AJ	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 11 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AK	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 12 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AL	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 13 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AM	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 14 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AN	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 15 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AO	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 16 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AP	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 17 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AQ	65	Total	C	N	O	S	0	0
			535	339	100	95	1		

- Molecule 18 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AR	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 19 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AS	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 20 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AT	65	Total	C	N	O	S	0	0
			544	335	117	91	1		

- Molecule 21 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	B0	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 22 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	B1	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 23 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	B2	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 24 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	B3	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 25 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	B5	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 26 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	B6	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 27 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	B7	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 28 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	B8	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 29 is a protein called Large ribosomal subunit protein bL36A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	B9	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 30 is a protein called Large ribosomal subunit protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	BA	134	Total	C	N	O	S	0	0
			1026	645	186	193	2		

- Molecule 31 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	BB	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 32 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	BC	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 33 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BD	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 34 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BE	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 35 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BF	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 36 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BI	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 37 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BK	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 38 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BM	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 39 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BN	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 40 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BO	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 41 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BP	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 42 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BQ	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 43 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BR	116	Total	C	N	O		0	0
			892	552	178	162			

- Molecule 44 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BS	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 45 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BT	117	Total	C	N	O		0	0
			947	604	192	151			

- Molecule 46 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BU	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 47 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BV	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 48 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BW	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 49 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	BX	102	Total	C	N	O	0	0
			779	492	146	141		

- Molecule 50 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BY	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 51 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	D1	1539	Total	C	N	O	P	0	0
			33012	14725	6052	10697	1538		

- Molecule 52 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	D2	2903	Total	C	N	O	P	0	0
			62317	27801	11468	20146	2902		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D2	747	C	U	conflict	GB CP194060.1

- Molecule 53 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	D3	120	Total	C	N	O	P	0	0
			2568	1145	471	833	119		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D3	120	A	U	conflict	GB CP076697.1

- Molecule 54 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	D4	7	Total	C	N	O	P	0	0
			153	69	32	45	7		

- Molecule 55 is a RNA chain called tRNA^fMet.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	D5	78	Total	C	N	O	P	S	0	0
			1650	738	298	537	76	1		

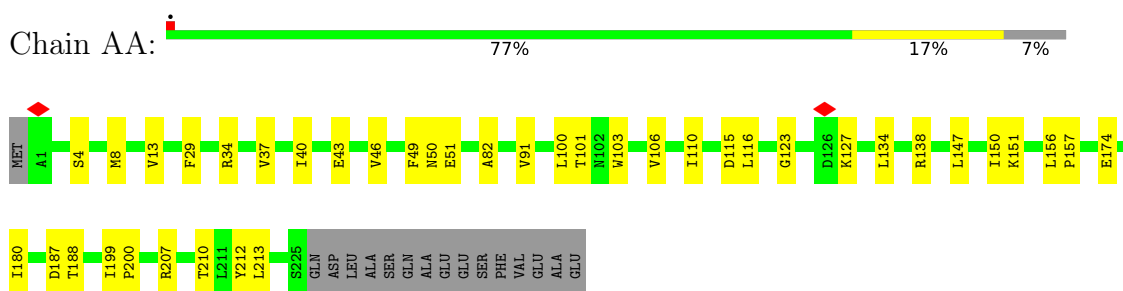
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D5	77	FME	A	conflict	GB CP194060.1

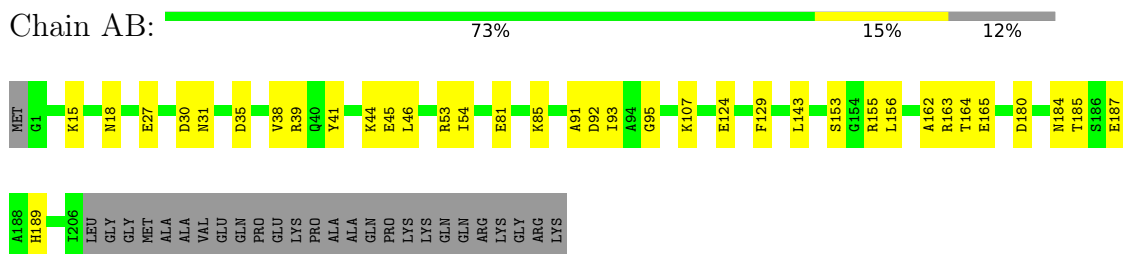
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

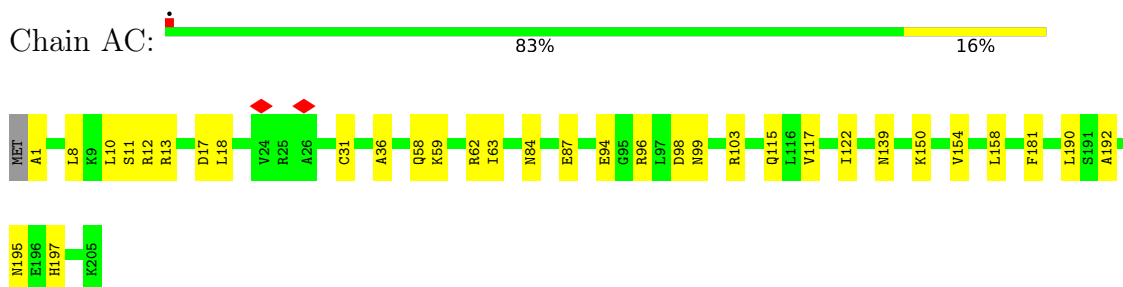
- Molecule 1: Small ribosomal subunit protein uS2



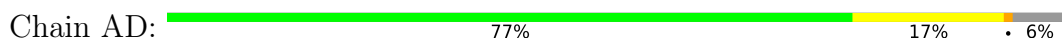
- Molecule 2: Small ribosomal subunit protein uS3

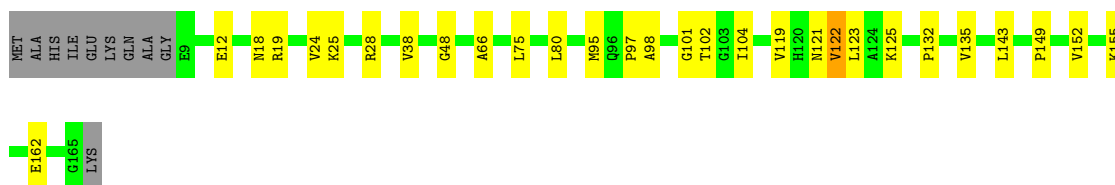


- Molecule 3: Small ribosomal subunit protein uS4



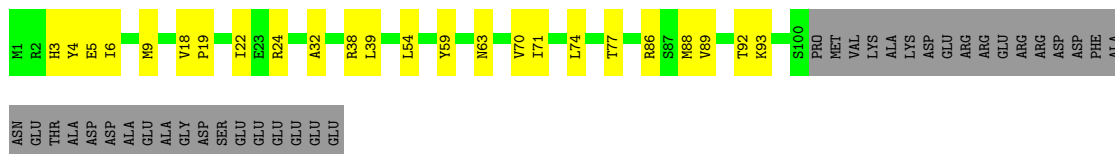
- Molecule 4: Small ribosomal subunit protein uS5





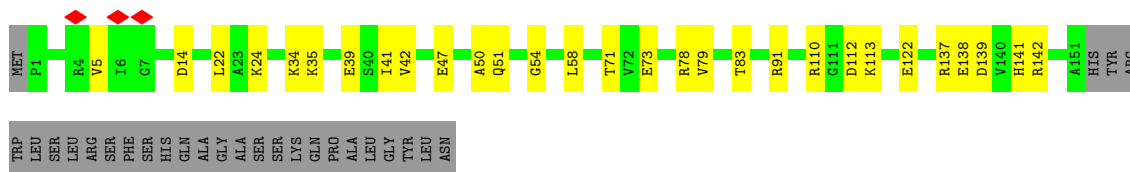
- Molecule 5: Small ribosomal subunit protein bS6, fully modified isoform

Chain AE: 56% 18% 26%



- Molecule 6: Small ribosomal subunit protein uS7

Chain AF: 68% 16% 16%



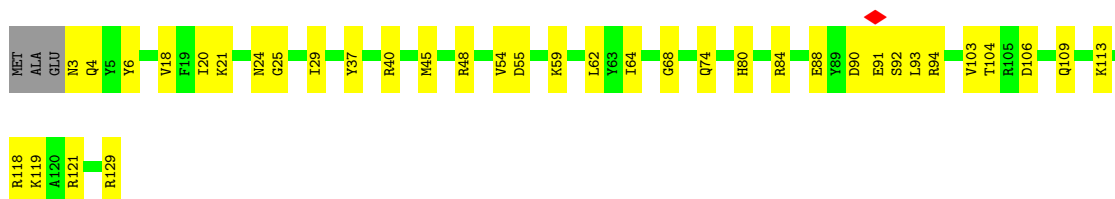
- Molecule 7: Small ribosomal subunit protein uS8

Chain AG: 75% 24% .



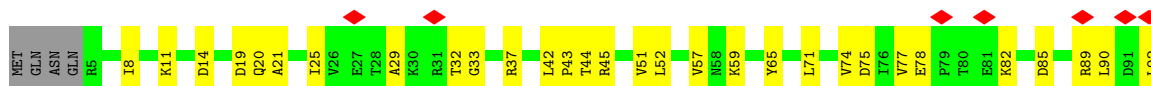
- Molecule 8: Small ribosomal subunit protein uS9

Chain AH: 69% 28% .



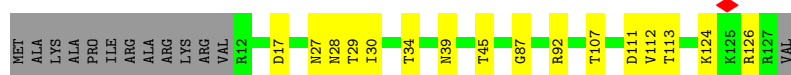
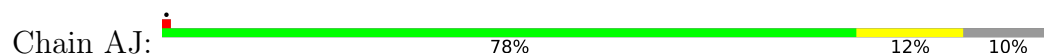
- Molecule 9: Small ribosomal subunit protein uS10

Chain AI: 7% 63% 32% 5%

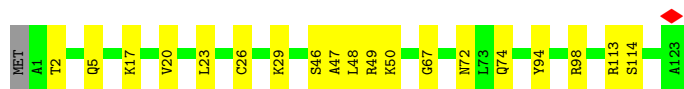
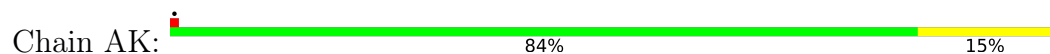




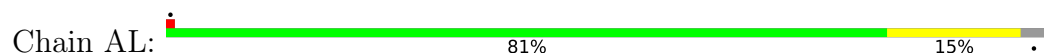
- Molecule 10: Small ribosomal subunit protein uS11



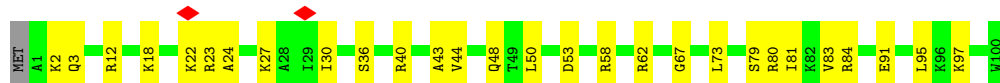
- Molecule 11: Small ribosomal subunit protein uS12



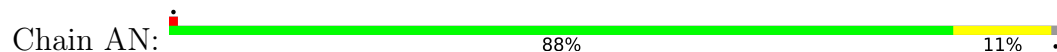
- Molecule 12: Small ribosomal subunit protein uS13



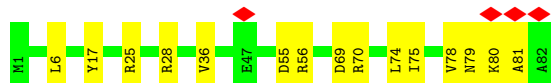
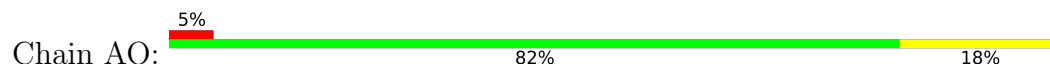
- Molecule 13: Small ribosomal subunit protein uS14



- Molecule 14: Small ribosomal subunit protein uS15



- Molecule 15: Small ribosomal subunit protein bS16



- Molecule 16: Small ribosomal subunit protein uS17

Chain AP:  73% 23% 5%



- Molecule 17: Small ribosomal subunit protein bS18

Chain AQ:  71% 16% 13%



- Molecule 18: Small ribosomal subunit protein uS19

Chain AR:  72% 14% 14%



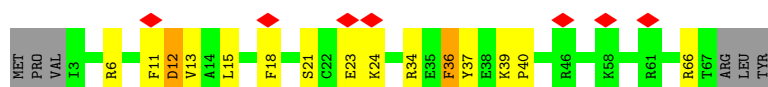
- Molecule 19: Small ribosomal subunit protein bS20

Chain AS:  86% 11% 3%



- Molecule 20: Small ribosomal subunit protein bS21

Chain AT:  10% 70% 18% 8%



- Molecule 21: Large ribosomal subunit protein bL27

Chain B0:  75% 13% 12%



- Molecule 22: Large ribosomal subunit protein bL28

Chain B1:  73% 26% 1%



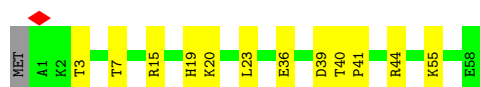
- Molecule 23: Large ribosomal subunit protein uL29

Chain B2:  87% 13%

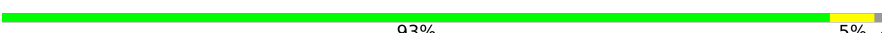


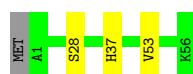
- Molecule 24: Large ribosomal subunit protein uL30

Chain B3:  78% 20%



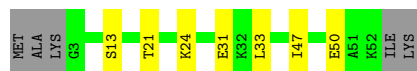
- Molecule 25: Large ribosomal subunit protein bL32

Chain B5:  93% 5%



- Molecule 26: Large ribosomal subunit protein bL33

Chain B6:  78% 13% 9%



- Molecule 27: Large ribosomal subunit protein bL34

Chain B7:  91% 9%

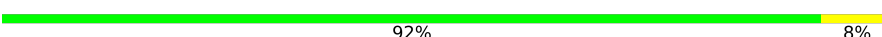


- Molecule 28: Large ribosomal subunit protein bL35

Chain B8:  88% 11%



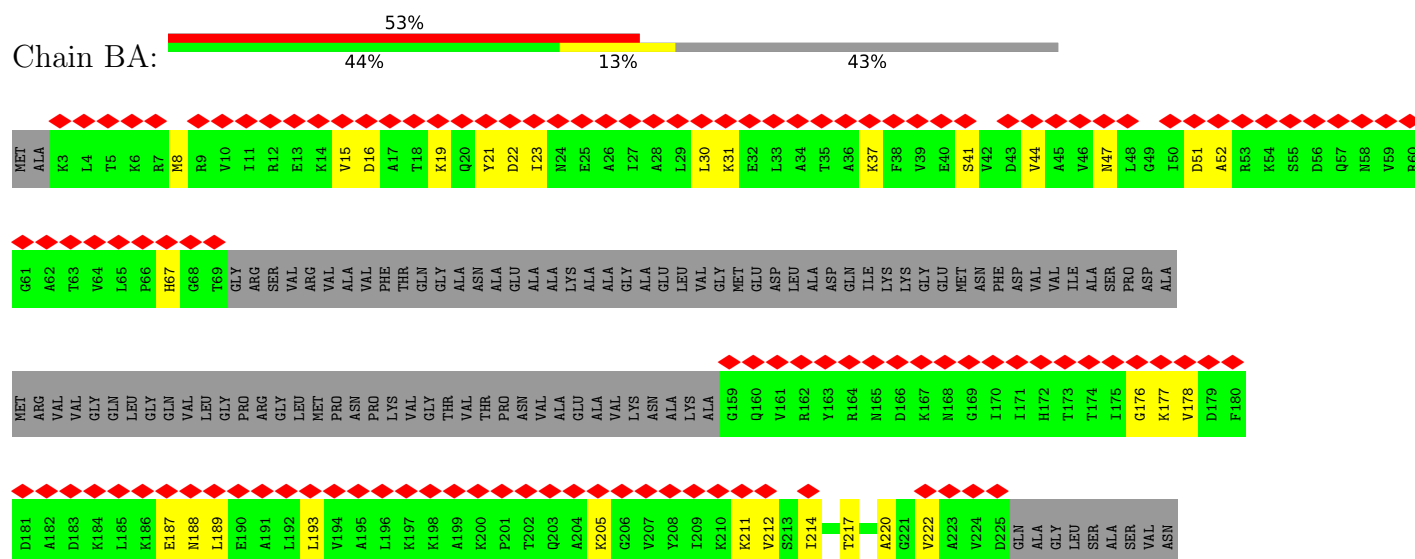
- Molecule 29: Large ribosomal subunit protein bL36A

Chain B9:  92% 8%



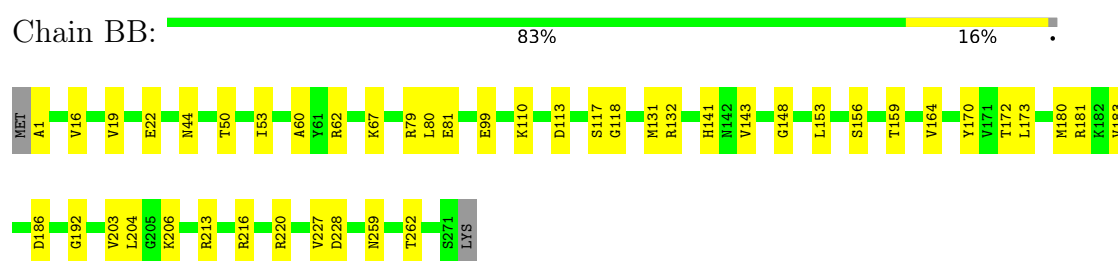
- Molecule 30: Large ribosomal subunit protein uL1

Chain BA:



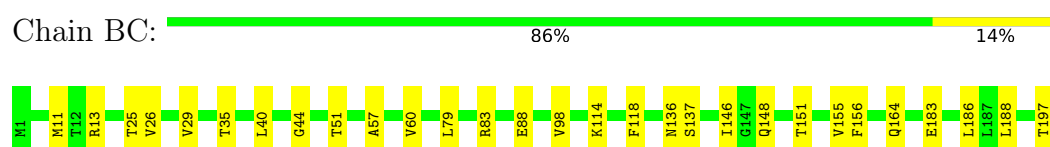
- Molecule 31: Large ribosomal subunit protein uL2

Chain BB:



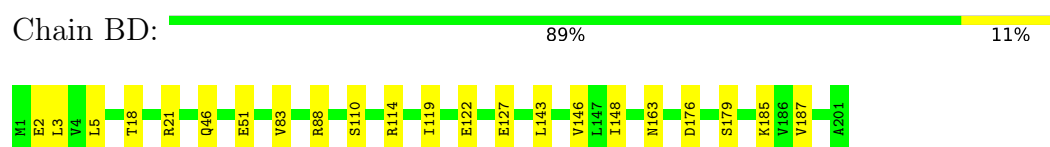
- Molecule 32: 50S ribosomal protein L3

Chain BC:



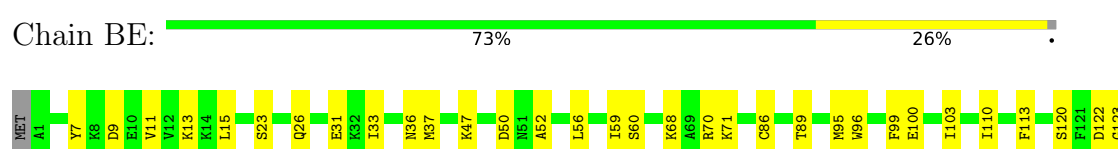
- Molecule 33: Large ribosomal subunit protein uL4

Chain BD:



- Molecule 34: Large ribosomal subunit protein uL5

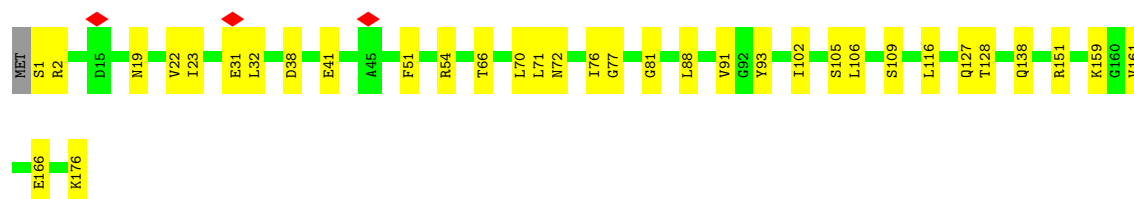
Chain BE:





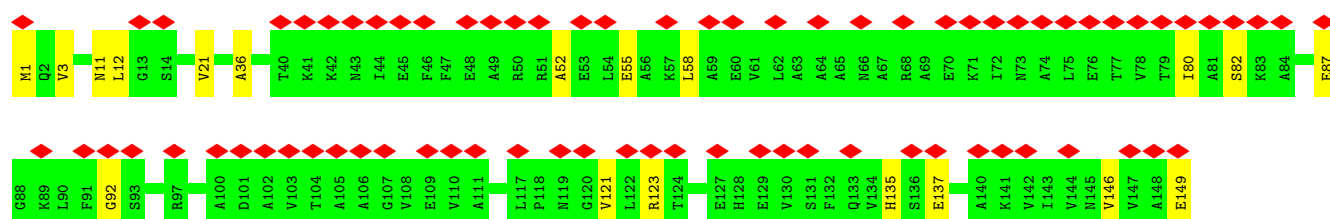
- Molecule 35: Large ribosomal subunit protein uL6

Chain BF: 80% 19%



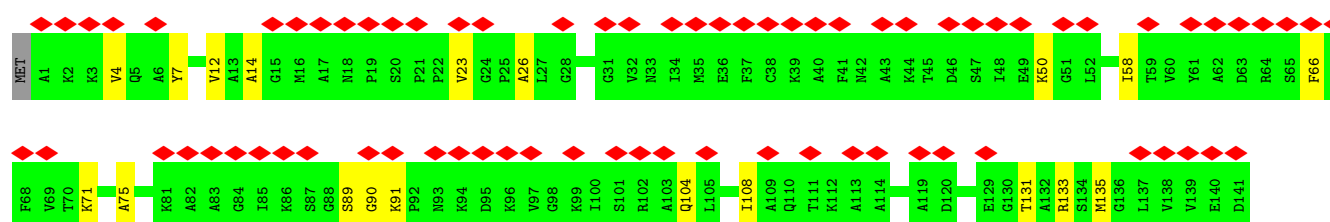
- Molecule 36: Large ribosomal subunit protein bL9

Chain BI: 50% 87% 13%



- Molecule 37: 50S ribosomal protein L11

Chain BK: 52% 86% 13%



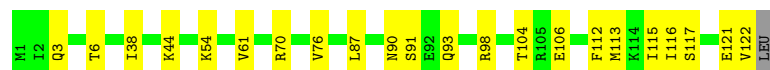
- Molecule 38: Large ribosomal subunit protein uL13

Chain BM: 88% 12%



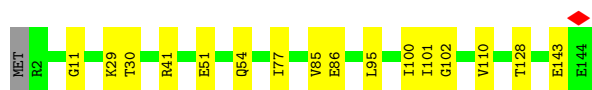
- Molecule 39: Large ribosomal subunit protein uL14

Chain BN: 81% 18%



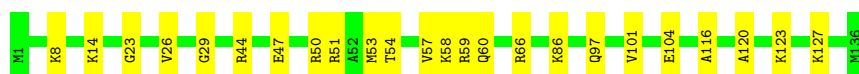
- Molecule 40: Large ribosomal subunit protein uL15

Chain BO:  88% 11%



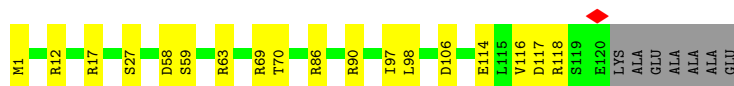
- Molecule 41: 50S ribosomal protein L16

Chain BP:  82% 18%



- Molecule 42: Large ribosomal subunit protein bL17

Chain BQ:  80% 14% 6%



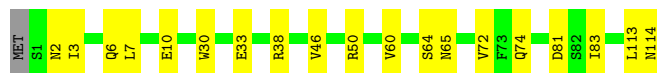
- Molecule 43: Large ribosomal subunit protein uL18

Chain BR:  91% 8% ..



- Molecule 44: Large ribosomal subunit protein bL19

Chain BS:  83% 17%



- Molecule 45: Large ribosomal subunit protein bL20

Chain BT:  86% 13%



- Molecule 46: Large ribosomal subunit protein bL21

Chain BU:  83% 16%



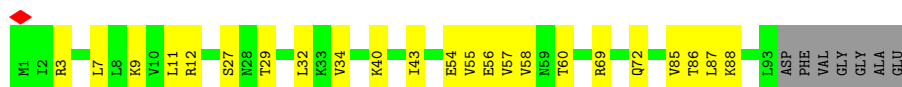
- Molecule 47: Large ribosomal subunit protein uL22

Chain BV:  80% 20%



- Molecule 48: Large ribosomal subunit protein uL23

Chain BW:  70% 23% 7%



- Molecule 49: Large ribosomal subunit protein uL24

Chain BX:  88% 11% .



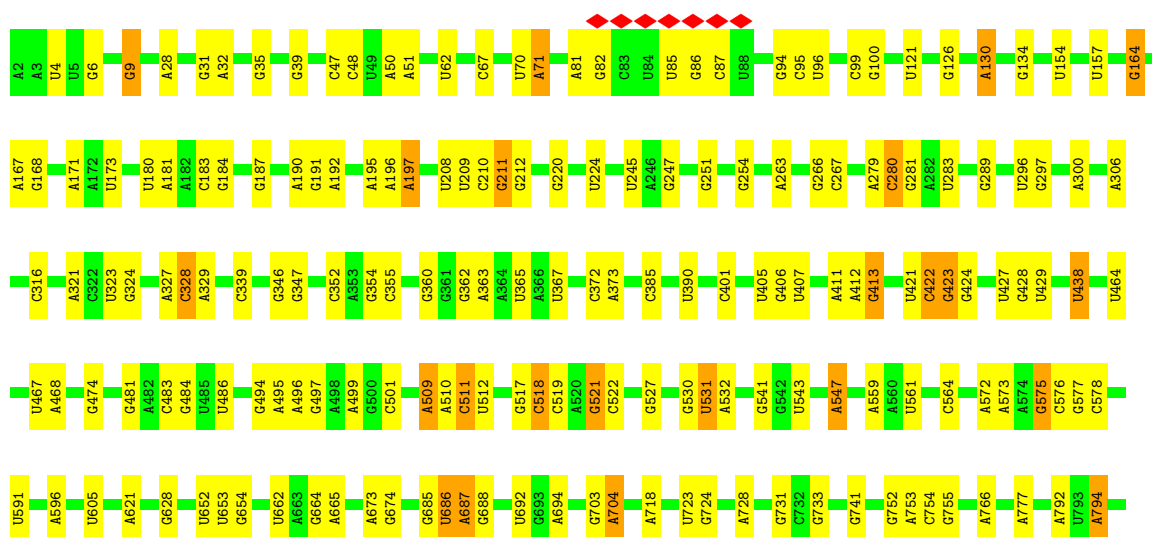
- Molecule 50: Large ribosomal subunit protein bL25

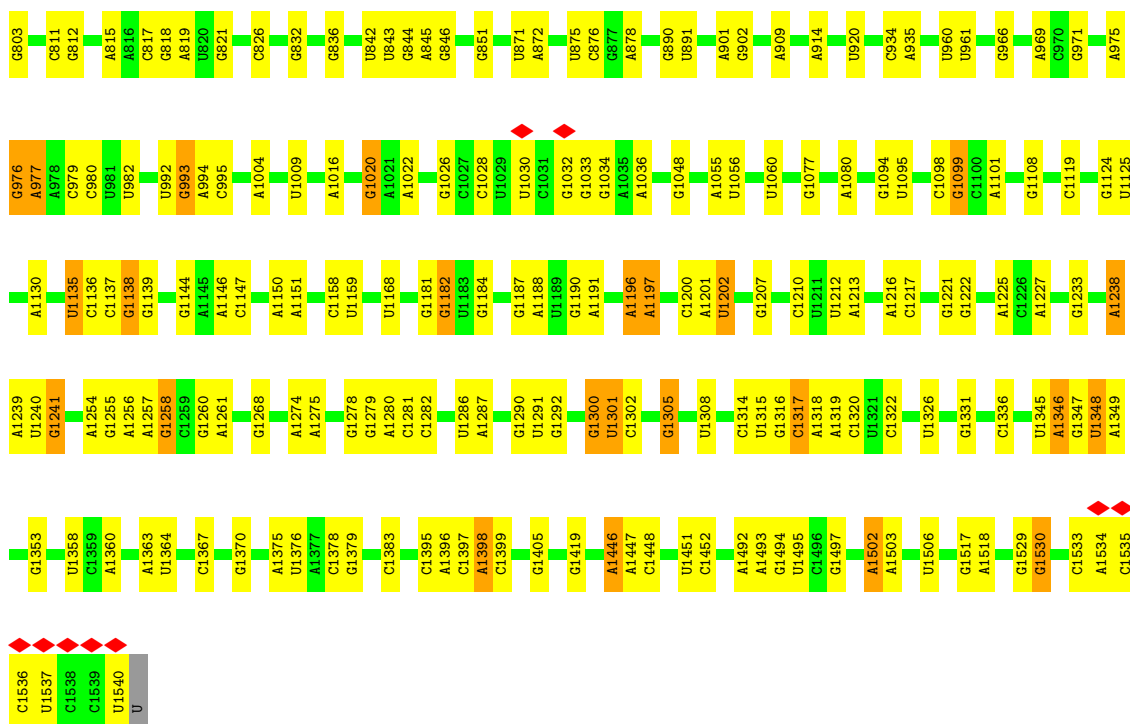
Chain BY:  83% 17%



- Molecule 51: 16S Ribosomal RNA

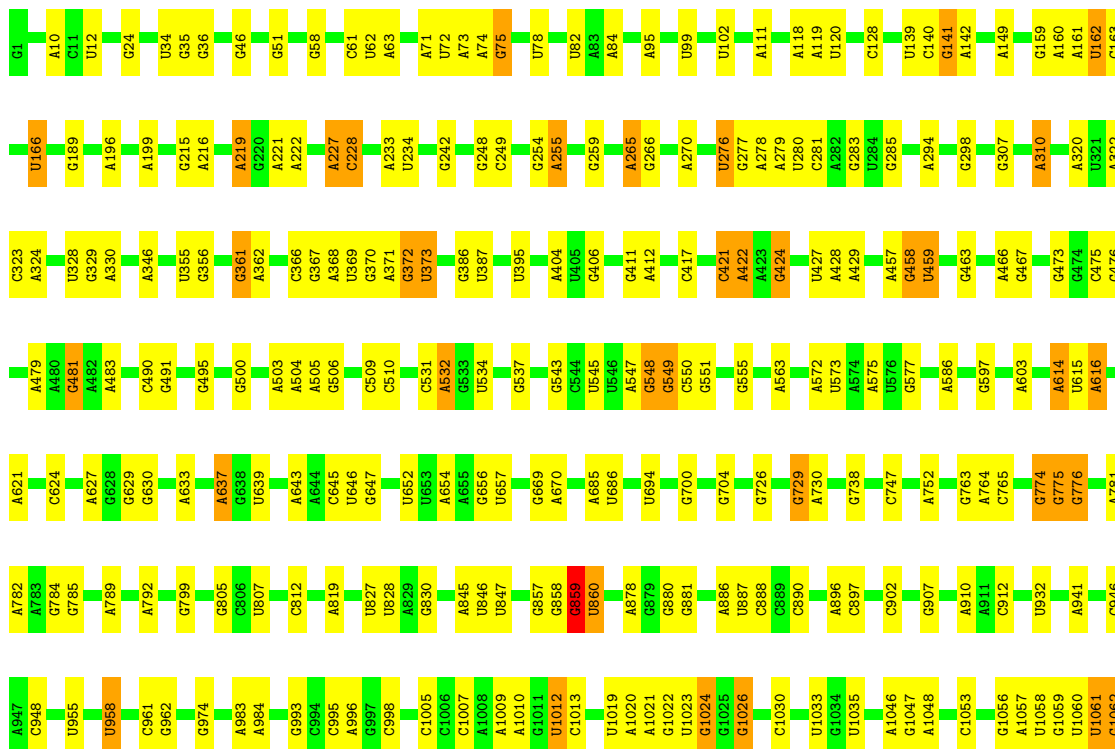
Chain D1:  75% 22% .

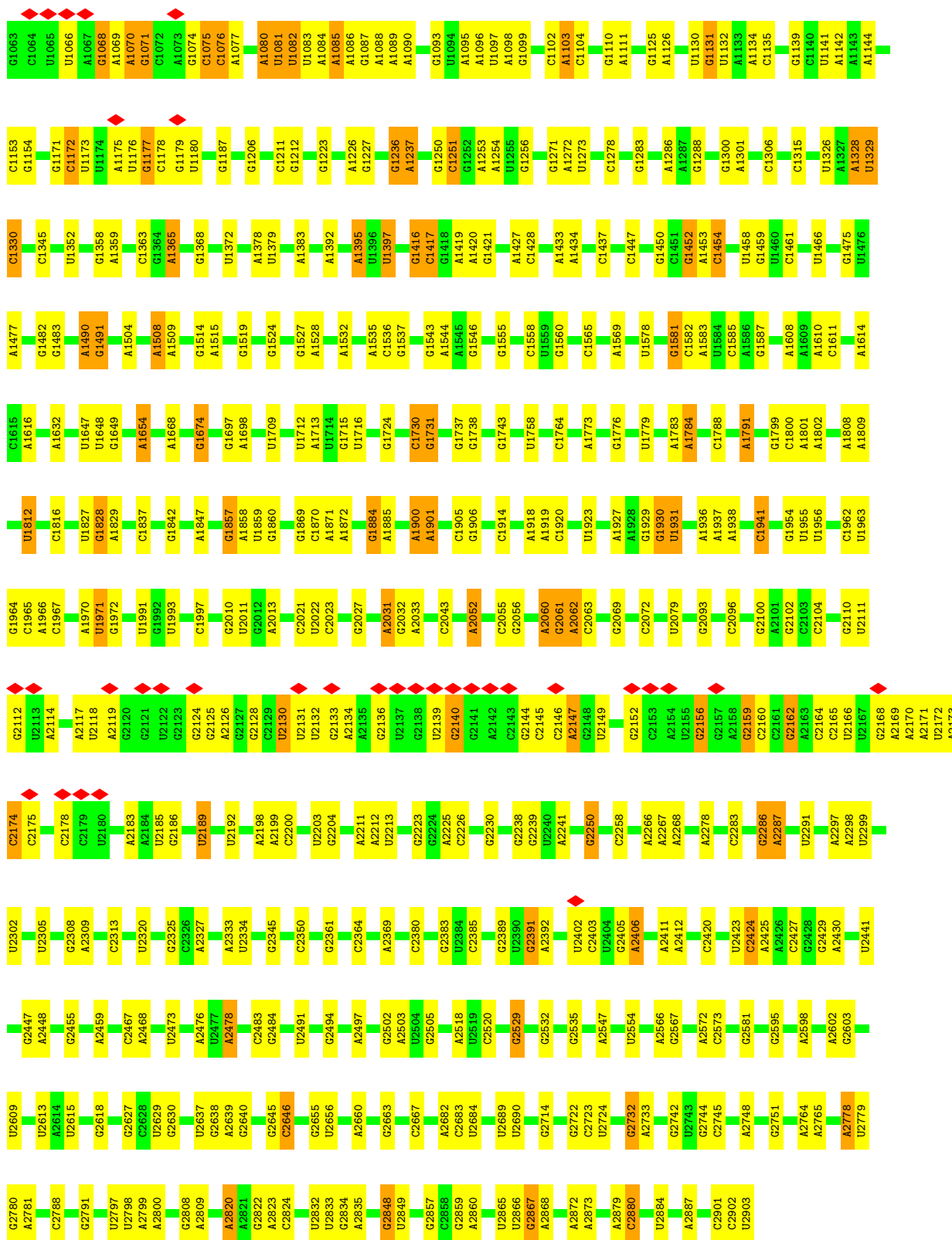




• Molecule 52: 23S Ribosomal RNA

Chain D2: 74% 22%





• Molecule 53: 5S Ribosomal RNA

Chain D3:

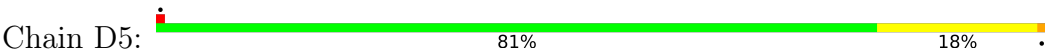




• Molecule 54: mRNA



• Molecule 55: tRNAfMet



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	31752	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	20.836	Depositor
Minimum map value	-6.791	Depositor
Average map value	0.010	Depositor
Map value standard deviation	1.097	Depositor
Recommended contour level	2.4	Depositor
Map size ($\text{\AA}$)	400.32, 400.32, 400.32	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.834, 0.834, 0.834	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FME

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AA	0.15	0/1787	0.36	0/2408
2	AB	0.18	0/1651	0.34	0/2225
3	AC	0.18	0/1665	0.37	0/2227
4	AD	0.19	0/1169	0.40	0/1573
5	AE	0.21	0/835	0.47	0/1128
6	AF	0.19	0/1195	0.45	0/1602
7	AG	0.20	0/989	0.40	0/1326
8	AH	0.17	0/1034	0.41	0/1375
9	AI	0.22	0/796	0.55	0/1077
10	AJ	0.19	0/885	0.39	0/1195
11	AK	0.21	0/969	0.39	0/1300
12	AL	0.18	0/892	0.37	0/1193
13	AM	0.19	0/817	0.39	0/1088
14	AN	0.20	0/722	0.38	0/964
15	AO	0.20	0/659	0.36	0/884
16	AP	0.19	0/657	0.46	0/881
17	AQ	0.18	0/544	0.35	0/731
18	AR	0.20	0/652	0.42	0/877
19	AS	0.19	0/671	0.39	0/888
20	AT	0.23	0/550	0.63	0/728
21	B0	0.19	0/582	0.29	0/769
22	B1	0.24	0/635	0.41	0/848
23	B2	0.20	0/510	0.44	0/677
24	B3	0.21	0/453	0.40	0/605
25	B5	0.21	0/450	0.42	0/599
26	B6	0.19	0/416	0.36	0/554
27	B7	0.24	0/380	0.33	0/498
28	B8	0.21	0/513	0.40	0/676
29	B9	0.23	0/303	0.44	0/397
30	BA	0.12	0/1033	0.29	0/1387
31	BB	0.22	0/2121	0.35	0/2852
32	BC	0.20	0/1586	0.34	0/2134

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	BD	0.18	0/1571	0.34	0/2113
34	BE	0.19	0/1434	0.43	0/1926
35	BF	0.16	0/1343	0.35	0/1816
36	BI	0.14	0/1122	0.36	0/1515
37	BK	0.18	0/1046	0.37	0/1410
38	BM	0.21	0/1152	0.34	0/1551
39	BN	0.21	0/947	0.37	0/1268
40	BO	0.18	0/1054	0.36	0/1403
41	BP	0.22	0/1093	0.39	0/1460
42	BQ	0.20	0/973	0.38	0/1301
43	BR	0.17	0/902	0.40	0/1209
44	BS	0.21	0/929	0.34	0/1242
45	BT	0.22	0/960	0.35	0/1278
46	BU	0.20	0/829	0.43	0/1107
47	BV	0.21	0/864	0.38	0/1156
48	BW	0.20	0/744	0.42	0/994
49	BX	0.18	0/787	0.37	0/1051
50	BY	0.19	0/766	0.36	0/1025
51	D1	0.20	0/36963	0.29	0/57662
52	D2	0.23	0/69796	0.31	1/108888 (0.0%)
53	D3	0.21	0/2872	0.29	0/4479
54	D4	0.11	0/172	0.21	0/266
55	D5	0.15	0/1832	0.25	0/2855
All	All	0.21	0/158272	0.32	1/236641 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	D2	859	G	C2'-C3'-O3'	5.05	117.07	109.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	1756	0	1787	25	0
2	AB	1624	0	1699	22	0
3	AC	1643	0	1710	20	0
4	AD	1156	0	1199	23	0
5	AE	817	0	808	18	0
6	AF	1181	0	1240	22	0
7	AG	979	0	1034	24	0
8	AH	1022	0	1070	27	0
9	AI	786	0	828	23	0
10	AJ	869	0	878	11	0
11	AK	955	0	1019	16	0
12	AL	883	0	944	11	0
13	AM	805	0	847	22	0
14	AN	714	0	737	6	0
15	AO	649	0	666	9	0
16	AP	648	0	691	14	0
17	AQ	535	0	552	8	0
18	AR	637	0	665	8	0
19	AS	665	0	714	6	0
20	AT	544	0	579	14	0
21	B0	575	0	592	7	0
22	B1	625	0	655	16	0
23	B2	509	0	543	6	0
24	B3	449	0	491	6	0
25	B5	444	0	461	2	0
26	B6	409	0	440	4	0
27	B7	377	0	418	3	0
28	B8	504	0	574	6	0
29	B9	302	0	343	4	0
30	BA	1026	0	1092	18	0
31	BB	2082	0	2157	28	0
32	BC	1565	0	1616	27	0
33	BD	1552	0	1619	14	0
34	BE	1410	0	1447	35	0
35	BF	1323	0	1374	23	0
36	BI	1111	0	1148	13	0
37	BK	1032	0	1088	18	0
38	BM	1129	0	1162	16	0
39	BN	938	0	1012	21	0
40	BO	1045	0	1117	12	0
41	BP	1074	0	1157	20	0
42	BQ	960	0	1000	14	0
43	BR	892	0	923	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	BS	917	0	965	16	0
45	BT	947	0	1022	13	0
46	BU	816	0	839	13	0
47	BV	857	0	922	19	0
48	BW	738	0	807	17	0
49	BX	779	0	834	7	0
50	BY	753	0	780	12	0
51	D1	33012	0	16618	141	0
52	D2	62317	0	31346	265	0
53	D3	2568	0	1303	11	0
54	D4	153	0	77	0	0
55	D5	1650	0	846	5	0
All	All	145708	0	98455	981	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (981) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:AR:35:ARG:NH2	51:D1:1221:G:OP1	2.07	0.88
8:AH:6:TYR:HH	51:D1:1147:C:HO2'	1.21	0.86
41:BP:58:LYS:O	41:BP:59:ARG:NE	2.09	0.85
37:BK:89:SER:OG	37:BK:135:MET:SD	2.35	0.84
13:AM:27:LYS:NZ	51:D1:1317:C:OP2	2.09	0.84
51:D1:1300:G:O2'	51:D1:1301:U:O5'	1.96	0.84
45:BT:48:ASP:OD2	52:D2:534:U:O2'	1.96	0.83
9:AI:42:LEU:HD22	9:AI:71:LEU:HD11	1.59	0.83
52:D2:2130:U:O2'	52:D2:2159:G:N2	2.13	0.82
39:BN:98:ARG:NH2	51:D1:339:C:OP1	2.12	0.82
52:D2:1858:A:N6	52:D2:1884:G:O2'	2.13	0.81
52:D2:859:G:OP1	52:D2:2268:A:O2'	1.98	0.81
52:D2:2857:G:N2	52:D2:2860:A:OP2	2.15	0.81
42:BQ:69:ARG:O	42:BQ:70:THR:OG1	1.99	0.80
52:D2:481:G:O2'	52:D2:506:G:N2	2.15	0.80
4:AD:155:LYS:NZ	7:AG:72:GLU:OE2	2.14	0.79
11:AK:113:ARG:NH2	51:D1:501:C:OP1	2.14	0.79
11:AK:50:LYS:NZ	51:D1:521:G:OP2	2.14	0.79
52:D2:270:A:N1	52:D2:369:U:O2'	2.14	0.79
21:B0:52:ASP:OD2	21:B0:54:THR:OG1	1.99	0.79
52:D2:1709:U:O2	52:D2:2859:G:N2	2.16	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:D2:1869:G:N2	52:D2:1872:A:OP2	2.16	0.79
34:BE:122:ASP:O	52:D2:2302:U:O2'	2.00	0.79
36:BI:52:ALA:N	36:BI:55:GLU:OE2	2.16	0.79
52:D2:1827:U:OP1	52:D2:1971:U:O2'	2.01	0.79
51:D1:1315:U:O2'	51:D1:1360:A:N3	2.14	0.78
51:D1:1135:U:O2'	51:D1:1138:G:O6	2.01	0.78
20:AT:6:ARG:O	20:AT:6:ARG:NH1	2.16	0.78
4:AD:121:ASN:O	4:AD:122:VAL:HG22	1.84	0.78
37:BK:71:LYS:NZ	52:D2:1059:G:OP1	2.16	0.78
39:BN:76:VAL:HG22	44:BS:72:VAL:HG22	1.63	0.77
31:BB:204:LEU:HD11	31:BB:213:ARG:HE	1.47	0.77
42:BQ:106:ASP:OD2	52:D2:1649:G:O2'	2.01	0.77
38:BM:49:ASP:OD1	38:BM:121:LYS:NZ	2.16	0.77
26:B6:33:LEU:N	26:B6:50:GLU:OE2	2.17	0.77
16:AP:48:GLU:OE1	16:AP:49:ASN:ND2	2.17	0.77
9:AI:77:VAL:HG23	9:AI:78:GLU:OE1	1.85	0.77
29:B9:2:LYS:NZ	52:D2:2478:A:OP2	2.14	0.77
41:BP:66:ARG:NH1	41:BP:104:GLU:OE2	2.18	0.77
52:D2:1466:U:HO2'	52:D2:1546:G:HO2'	1.30	0.77
41:BP:14:LYS:NZ	52:D2:958:U:OP2	2.18	0.76
30:BA:41:SER:OG	30:BA:176:GLY:O	2.02	0.76
52:D2:475:C:O2	52:D2:479:A:N6	2.18	0.76
52:D2:859:G:O2'	52:D2:860:U:OP2	2.04	0.76
15:AO:25:ARG:NH1	51:D1:134:G:O6	2.18	0.76
15:AO:75:ILE:O	15:AO:80:LYS:NZ	2.18	0.76
23:B2:58:ASN:ND2	52:D2:72:U:O4	2.19	0.76
51:D1:1255:G:O2'	51:D1:1258:G:N3	2.19	0.76
1:AA:50:ASN:OD1	1:AA:51:GLU:N	2.17	0.76
42:BQ:86:ARG:NE	42:BQ:117:ASP:OD2	2.18	0.76
22:B1:32:LEU:HD21	22:B1:49:ARG:HG2	1.65	0.76
2:AB:27:GLU:N	2:AB:27:GLU:OE1	2.19	0.76
52:D2:1528:A:OP2	52:D2:1543:G:N2	2.17	0.76
31:BB:170:TYR:OH	52:D2:2223:G:OP1	2.02	0.76
6:AF:137:ARG:NH1	6:AF:138:GLU:OE2	2.19	0.75
48:BW:56:GLU:OE1	48:BW:88:LYS:NZ	2.19	0.75
31:BB:259:ASN:ND2	31:BB:262:THR:OG1	2.18	0.75
5:AE:24:ARG:NH1	36:BI:87:GLU:OE2	2.20	0.74
18:AR:72:GLU:OE1	18:AR:72:GLU:N	2.20	0.74
40:BO:29:LYS:O	40:BO:30:THR:OG1	2.02	0.74
52:D2:285:G:O6	52:D2:355:U:O2	2.06	0.74
17:AQ:13:THR:OG1	17:AQ:16:GLY:O	2.05	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:B6:24:LYS:NZ	26:B6:31:GLU:O	2.19	0.74
35:BF:127:GLN:NE2	35:BF:128:THR:OG1	2.19	0.74
52:D2:1447:C:O2'	52:D2:1544:A:N3	2.21	0.74
10:AJ:124:LYS:O	20:AT:34:ARG:NH1	2.21	0.74
6:AF:110:ARG:NH2	6:AF:122:GLU:OE1	2.21	0.74
47:BV:4:ILE:HG22	47:BV:106:VAL:HG22	1.68	0.74
52:D2:2595:G:N2	52:D2:2598:A:OP2	2.21	0.74
35:BF:2:ARG:NH1	52:D2:2751:G:OP2	2.20	0.73
52:D2:141:G:N2	52:D2:141:G:OP2	2.21	0.73
51:D1:1405:G:O2'	51:D1:1518:A:O2'	2.06	0.73
52:D2:259:G:HO2'	52:D2:621:A:HO2'	1.31	0.73
52:D2:1417:C:HO2'	52:D2:1587:G:HO2'	1.31	0.73
13:AM:18:LYS:O	13:AM:22:LYS:NZ	2.22	0.73
8:AH:119:LYS:NZ	51:D1:1349:A:OP2	2.22	0.73
33:BD:21:ARG:O	33:BD:114:ARG:NH1	2.22	0.73
34:BE:89:THR:OG1	53:D3:42:C:N3	2.22	0.73
13:AM:2:LYS:NZ	51:D1:1216:A:OP1	2.14	0.72
34:BE:47:LYS:NZ	34:BE:50:ASP:OD2	2.22	0.72
4:AD:28:ARG:NH2	51:D1:1397:C:OP2	2.22	0.72
32:BC:146:ILE:HD12	32:BC:155:VAL:HG11	1.71	0.72
41:BP:47:GLU:OE1	41:BP:51:ARG:NH1	2.22	0.71
44:BS:33:GLU:OE1	44:BS:33:GLU:N	2.23	0.71
52:D2:776:G:N2	52:D2:2241:A:OP1	2.22	0.71
52:D2:1900:A:O2'	52:D2:1901:A:OP2	2.07	0.71
2:AB:124:GLU:OE2	2:AB:189:HIS:N	2.23	0.71
51:D1:1016:A:O2'	51:D1:1217:C:O2'	2.07	0.71
52:D2:1125:G:OP2	52:D2:1126:A:O2'	2.04	0.71
40:BO:51:GLU:OE1	40:BO:54:GLN:NE2	2.23	0.71
8:AH:118:ARG:NH1	51:D1:1233:G:OP1	2.24	0.71
52:D2:227:A:O2'	52:D2:228:C:O5'	2.08	0.71
52:D2:1081:U:C4	52:D2:1082:U:O4	2.44	0.70
51:D1:1077:G:N2	51:D1:1080:A:OP2	2.21	0.70
52:D2:1173:U:O2	52:D2:1177:G:N1	2.24	0.70
1:AA:110:ILE:HD13	1:AA:147:LEU:HD21	1.74	0.70
19:AS:10:ALA:O	19:AS:13:SER:OG	2.10	0.70
35:BF:176:LYS:NZ	52:D2:2660:A:N7	2.39	0.70
52:D2:1962:C:O2'	52:D2:1964:G:OP2	2.10	0.70
51:D1:1009:U:O2	51:D1:1020:G:O6	2.09	0.70
33:BD:46:GLN:O	33:BD:88:ARG:NH2	2.25	0.70
45:BT:83:LYS:NZ	52:D2:998:C:OP1	2.24	0.70
52:D2:1936:A:N6	52:D2:1963:U:O2	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AF:91:ARG:NH2	51:D1:1378:C:O2'	2.25	0.70
9:AI:32:THR:OG1	9:AI:82:LYS:NZ	2.22	0.70
52:D2:2406:A:OP2	52:D2:2411:A:N6	2.24	0.69
52:D2:1315:C:O2'	52:D2:1392:A:N3	2.23	0.69
3:AC:59:LYS:O	3:AC:63:ILE:HD12	1.91	0.69
52:D2:774:G:O2'	52:D2:775:G:O5'	2.08	0.69
41:BP:8:LYS:NZ	52:D2:912:C:OP1	2.25	0.69
34:BE:36:ASN:ND2	52:D2:2313:C:O4'	2.26	0.69
52:D2:643:A:N1	52:D2:2369:A:O2'	2.25	0.69
52:D2:2865:U:OP2	52:D2:2866:U:O2'	2.05	0.69
8:AH:88:GLU:OE1	8:AH:88:GLU:N	2.25	0.68
13:AM:79:SER:O	13:AM:83:VAL:HG23	1.93	0.68
51:D1:180:U:O2	51:D1:195:A:N7	2.26	0.68
28:B8:28:LEU:O	28:B8:28:LEU:HD12	1.93	0.68
51:D1:1316:G:N1	51:D1:1319:A:OP2	2.26	0.67
51:D1:28:A:O2'	51:D1:296:U:OP1	2.12	0.67
51:D1:321:A:N6	51:D1:328:C:O2'	2.28	0.67
6:AF:139:ASP:OD1	6:AF:142:ARG:NH2	2.27	0.67
51:D1:195:A:O2'	51:D1:196:A:O4'	2.11	0.67
37:BK:133:ARG:NH1	52:D2:1077:A:O2'	2.28	0.67
51:D1:792:A:O2'	51:D1:794:A:N7	2.26	0.67
52:D2:2646:C:OP2	52:D2:2732:G:O2'	2.13	0.67
2:AB:18:ASN:OD1	2:AB:53:ARG:NH2	2.28	0.67
5:AE:5:GLU:OE2	17:AQ:23:LYS:NZ	2.20	0.67
6:AF:34:LYS:NZ	51:D1:1241:G:OP2	2.28	0.67
34:BE:133:GLU:OE1	34:BE:135:ILE:HG22	1.95	0.67
51:D1:401:C:O2'	51:D1:621:A:N3	2.27	0.66
41:BP:23:GLY:O	41:BP:101:VAL:HG22	1.95	0.66
46:BU:16:GLU:OE2	46:BU:17:GLY:N	2.28	0.66
52:D2:2139:U:O2	52:D2:2152:G:O6	2.13	0.66
3:AC:96:ARG:NH2	3:AC:98:ASP:OD1	2.27	0.66
31:BB:1:ALA:N	31:BB:19:VAL:O	2.28	0.66
52:D2:1061:U:O2'	52:D2:1070:A:O4'	2.13	0.66
2:AB:81:GLU:OE1	2:AB:85:LYS:NZ	2.28	0.66
52:D2:307:G:N1	52:D2:310:A:OP2	2.29	0.66
49:BX:56:GLY:N	52:D2:483:A:O2'	2.29	0.65
31:BB:181:ARG:NH2	52:D2:1799:G:O3'	2.29	0.65
45:BT:49:ARG:O	45:BT:53:LYS:NZ	2.29	0.65
22:B1:2:ARG:NH1	52:D2:1365:A:OP1	2.29	0.65
51:D1:686:U:O2'	51:D1:687:A:O5'	2.14	0.65
52:D2:1954:G:O2'	52:D2:1956:U:O4	2.08	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AG:9:MET:O	7:AG:13:ILE:HD12	1.97	0.65
11:AK:17:LYS:NZ	51:D1:909:A:OP1	2.28	0.65
26:B6:13:SER:OG	26:B6:47:ILE:O	2.11	0.65
36:BI:1:MET:N	36:BI:21:VAL:O	2.28	0.65
35:BF:38:ASP:O	35:BF:54:ARG:NH1	2.30	0.65
44:BS:6:GLN:NE2	44:BS:10:GLU:OE2	2.30	0.65
13:AM:62:ARG:NH1	13:AM:67:GLY:O	2.29	0.65
24:B3:15:ARG:O	24:B3:20:LYS:NZ	2.28	0.65
43:BR:93:ASP:OD2	43:BR:95:SER:OG	2.09	0.65
47:BV:28:LYS:NZ	47:BV:31:GLN:OE1	2.30	0.65
34:BE:31:GLU:N	34:BE:31:GLU:OE1	2.30	0.65
51:D1:413:G:O2'	51:D1:428:G:N2	2.30	0.65
52:D2:700:G:O2'	52:D2:1632:A:N3	2.30	0.65
39:BN:3:GLN:O	39:BN:6:THR:OG1	2.13	0.64
39:BN:113:MET:O	39:BN:117:SER:OG	2.14	0.64
52:D2:2788:C:O2'	52:D2:2809:A:N3	2.29	0.64
1:AA:82:ALA:HB2	1:AA:213:LEU:HD13	1.80	0.64
39:BN:38:ILE:CD1	39:BN:61:VAL:HG22	2.27	0.64
51:D1:1261:A:N6	51:D1:1274:A:O2'	2.30	0.64
7:AG:30:LYS:NZ	51:D1:591:U:OP1	2.24	0.64
52:D2:1056:G:O2'	52:D2:1103:A:N6	2.30	0.64
8:AH:40:ARG:NH2	51:D1:1292:G:OP1	2.28	0.64
30:BA:30:LEU:HD13	30:BA:178:VAL:HB	1.78	0.64
34:BE:161:SER:OG	34:BE:164:GLU:OE1	2.15	0.64
39:BN:70:ARG:NH1	52:D2:2684:U:O4'	2.30	0.64
51:D1:530:G:O2'	51:D1:531:U:OP1	2.14	0.64
4:AD:95:MET:HE1	4:AD:143:LEU:HD12	1.80	0.64
51:D1:208:U:HO2'	51:D1:211:G:H1	1.45	0.64
52:D2:370:G:O2'	52:D2:424:G:OP1	2.15	0.64
30:BA:47:ASN:ND2	30:BA:211:LYS:O	2.31	0.64
36:BI:82:SER:O	36:BI:149:GLU:N	2.31	0.63
48:BW:9:LYS:O	48:BW:12:ARG:NH2	2.30	0.63
41:BP:127:LYS:NZ	52:D2:1030:C:OP2	2.31	0.63
50:BY:41:GLU:N	50:BY:41:GLU:OE1	2.31	0.63
52:D2:2164:C:OP2	52:D2:2165:C:N4	2.26	0.63
51:D1:71:A:N6	51:D1:99:C:O2'	2.27	0.63
2:AB:187:GLU:OE1	2:AB:187:GLU:N	2.31	0.63
5:AE:54:LEU:HD12	5:AE:54:LEU:O	1.99	0.63
3:AC:1:ALA:N	51:D1:405:U:O4	2.29	0.63
34:BE:135:ILE:HA	34:BE:140:ILE:HD11	1.81	0.63
41:BP:57:VAL:O	41:BP:60:GLN:NE2	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AM:97:LYS:NZ	51:D1:1188:A:O3'	2.31	0.63
16:AP:63:CYS:SG	16:AP:73:THR:HG23	2.38	0.63
51:D1:1238:A:N7	51:D1:1301:U:O4	2.30	0.63
12:AL:106:ARG:NH2	12:AL:110:GLY:O	2.31	0.63
20:AT:66:ARG:NH1	51:D1:1098:C:O2'	2.32	0.63
15:AO:69:ASP:OD1	15:AO:70:ARG:N	2.32	0.62
52:D2:1416:G:O2'	52:D2:1417:C:O5'	2.17	0.62
2:AB:162:ALA:N	51:D1:1056:U:OP1	2.33	0.62
52:D2:1070:A:O2'	52:D2:1097:U:OP1	2.08	0.62
52:D2:259:G:O2'	52:D2:621:A:O2'	2.05	0.62
40:BO:41:ARG:NH2	52:D2:807:U:OP2	2.31	0.62
1:AA:43:GLU:OE1	1:AA:43:GLU:N	2.32	0.62
52:D2:2144:G:O2'	52:D2:2147:A:N6	2.33	0.62
7:AG:90:GLU:N	7:AG:90:GLU:OE2	2.31	0.62
9:AI:29:ALA:O	9:AI:33:GLY:N	2.33	0.62
11:AK:114:SER:O	51:D1:35:G:O2'	2.14	0.62
28:B8:33:THR:HG23	52:D2:2420:C:OP1	1.99	0.62
9:AI:19:ASP:OD1	9:AI:20:GLN:N	2.32	0.62
23:B2:2:LYS:NZ	52:D2:78:U:OP1	2.23	0.62
7:AG:46:GLU:O	7:AG:61:THR:OG1	2.16	0.62
8:AH:40:ARG:NH1	51:D1:1291:U:O3'	2.33	0.62
52:D2:1477:A:N6	52:D2:1514:G:O2'	2.33	0.62
11:AK:67:GLY:O	11:AK:98:ARG:NH1	2.33	0.61
5:AE:74:LEU:O	5:AE:77:THR:OG1	2.18	0.61
9:AI:21:ALA:O	9:AI:25:ILE:HD12	2.01	0.61
49:BX:40:LEU:HD12	49:BX:59:GLU:OE2	2.01	0.61
9:AI:51:VAL:HG13	13:AM:80:ARG:HB2	1.83	0.61
12:AL:57:ASP:OD1	12:AL:58:GLU:N	2.33	0.61
31:BB:60:ALA:O	31:BB:62:ARG:NH1	2.33	0.61
39:BN:93:GLN:N	39:BN:93:GLN:OE1	2.33	0.61
49:BX:6:ARG:NH2	52:D2:99:U:O2	2.33	0.61
52:D2:1288:G:OP2	52:D2:1288:G:N2	2.25	0.61
19:AS:68:LYS:NZ	51:D1:224:U:OP1	2.33	0.61
30:BA:177:LYS:NZ	52:D2:2125:G:OP1	2.32	0.61
39:BN:90:ASN:OD1	39:BN:91:SER:N	2.33	0.61
50:BY:14:LYS:NZ	53:D3:79:G:O6	2.30	0.61
51:D1:422:C:O2'	51:D1:423:G:N2	2.33	0.61
14:AN:72:LYS:NZ	51:D1:753:A:OP1	2.33	0.61
46:BU:68:ARG:NH1	52:D2:1223:G:OP1	2.33	0.61
13:AM:73:LEU:HD12	13:AM:83:VAL:HG21	1.83	0.61
2:AB:163:ARG:NE	2:AB:165:GLU:OE2	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AF:24:LYS:NZ	51:D1:1376:U:OP2	2.34	0.60
32:BC:26:VAL:CG1	32:BC:186:LEU:HD11	2.31	0.60
41:BP:53:MET:HE1	41:BP:116:ALA:O	2.01	0.60
13:AM:36:SER:OG	13:AM:40:ARG:NH2	2.33	0.60
13:AM:84:ARG:NH2	51:D1:1060:U:OP1	2.34	0.60
37:BK:7:TYR:OH	52:D2:1099:G:OP1	2.09	0.60
51:D1:438:U:N3	51:D1:494:G:N7	2.49	0.60
33:BD:127:GLU:N	33:BD:127:GLU:OE1	2.34	0.60
39:BN:61:VAL:HG23	39:BN:87:LEU:CD1	2.32	0.60
30:BA:8:MET:HE1	52:D2:2174:C:H4'	1.82	0.60
32:BC:88:GLU:N	32:BC:88:GLU:OE1	2.34	0.60
32:BC:156:PHE:CD1	38:BM:81:ILE:HD11	2.36	0.60
11:AK:26:CYS:SG	51:D1:363:A:N6	2.75	0.60
32:BC:148:GLN:OE1	32:BC:148:GLN:N	2.35	0.60
36:BI:137:GLU:N	36:BI:137:GLU:OE1	2.34	0.60
43:BR:112:GLU:N	43:BR:112:GLU:OE1	2.34	0.60
51:D1:297:G:N2	51:D1:300:A:OP2	2.30	0.60
52:D2:1395:A:O2'	52:D2:1397:U:OP2	2.10	0.60
22:B1:32:LEU:HD21	22:B1:49:ARG:CG	2.31	0.60
32:BC:13:ARG:NH2	44:BS:74:GLN:OE1	2.35	0.60
3:AC:12:ARG:NH1	3:AC:36:ALA:O	2.34	0.60
31:BB:67:LYS:NZ	31:BB:148:GLY:O	2.35	0.60
52:D2:2405:G:O2'	52:D2:2412:A:N6	2.35	0.60
34:BE:122:ASP:OD1	34:BE:123:GLY:N	2.35	0.59
8:AH:18:VAL:HG12	8:AH:64:ILE:HD12	1.84	0.59
52:D2:1172:C:O2'	52:D2:1173:U:O4'	2.20	0.59
18:AR:4:LEU:HD23	18:AR:9:PHE:HB2	1.85	0.59
52:D2:2060:A:O2'	52:D2:2061:G:OP2	2.17	0.59
9:AI:85:ASP:O	9:AI:89:ARG:NH1	2.35	0.59
32:BC:151:THR:OG1	52:D2:2032:G:N2	2.36	0.59
34:BE:37:MET:HE3	34:BE:151:LEU:HD21	1.85	0.59
4:AD:18:ASN:OD1	4:AD:19:ARG:N	2.35	0.59
31:BB:99:GLU:OE1	52:D2:1491:G:O2'	2.21	0.59
32:BC:114:LYS:NZ	52:D2:2723:C:OP1	2.22	0.59
8:AH:54:VAL:HG11	8:AH:93:LEU:HD11	1.85	0.59
12:AL:43:LYS:N	12:AL:46:GLU:OE2	2.34	0.59
46:BU:4:VAL:O	46:BU:39:LEU:N	2.36	0.59
1:AA:29:PHE:O	1:AA:40:ILE:HG23	2.01	0.58
2:AB:129:PHE:CG	2:AB:156:LEU:HD12	2.38	0.58
8:AH:55:ASP:O	8:AH:59:LYS:NZ	2.20	0.58
52:D2:1923:U:OP1	55:D5:24:U:O2'	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:BB:164:VAL:HG11	31:BB:180:MET:HE1	1.84	0.58
52:D2:2291:U:OP1	52:D2:2380:C:O2'	2.20	0.58
4:AD:12:GLU:HG3	4:AD:38:VAL:HG22	1.85	0.58
10:AJ:30:ILE:HG12	10:AJ:45:THR:HG22	1.84	0.58
35:BF:77:GLY:O	35:BF:81:GLY:N	2.36	0.58
39:BN:76:VAL:HG22	44:BS:72:VAL:CG2	2.30	0.58
39:BN:112:PHE:HB3	39:BN:115:ILE:HD12	1.86	0.58
51:D1:1300:G:HO2'	51:D1:1301:U:P	2.26	0.58
22:B1:71:ARG:NH1	22:B1:77:TYR:OH	2.37	0.58
52:D2:219:A:N3	52:D2:234:U:O2'	2.34	0.58
33:BD:5:LEU:HD23	33:BD:122:GLU:CD	2.29	0.58
34:BE:56:LEU:HD12	34:BE:86:CYS:SG	2.44	0.58
52:D2:2134:A:C6	52:D2:2156:G:N2	2.72	0.58
52:D2:577:G:O2'	52:D2:1254:A:OP1	2.21	0.58
34:BE:37:MET:SD	34:BE:52:ALA:HB1	2.44	0.57
51:D1:321:A:N6	51:D1:328:C:HO2'	2.02	0.57
52:D2:1329:U:O2'	52:D2:1330:C:OP1	2.15	0.57
15:AO:28:ARG:NH2	51:D1:390:U:O3'	2.37	0.57
31:BB:216:ARG:NH2	52:D2:781:A:OP1	2.36	0.57
46:BU:54:VAL:HG22	46:BU:55:ASP:H	1.68	0.57
46:BU:55:ASP:OD1	46:BU:56:GLY:N	2.37	0.57
1:AA:115:ASP:OD1	1:AA:116:LEU:N	2.36	0.57
5:AE:6:ILE:HG22	5:AE:89:VAL:HG12	1.85	0.57
52:D2:2848:G:O2'	52:D2:2867:G:N2	2.35	0.57
2:AB:15:LYS:NZ	2:AB:180:ASP:OD1	2.24	0.57
8:AH:91:GLU:OE2	8:AH:94:ARG:NH1	2.38	0.57
36:BI:92:GLY:O	36:BI:123:ARG:NH1	2.37	0.57
52:D2:285:G:C6	52:D2:355:U:O2	2.57	0.57
3:AC:117:VAL:HG22	3:AC:122:ILE:HD13	1.87	0.57
8:AH:3:ASN:O	8:AH:21:LYS:NZ	2.26	0.57
12:AL:68:LEU:O	12:AL:72:ILE:HD12	2.04	0.57
8:AH:80:HIS:NE2	8:AH:103:VAL:O	2.37	0.57
35:BF:88:LEU:HB3	35:BF:161:VAL:HG12	1.86	0.57
41:BP:50:ARG:O	41:BP:54:THR:HG23	2.05	0.57
43:BR:94:ARG:NH1	43:BR:97:PHE:O	2.34	0.57
45:BT:57:ARG:NH1	52:D2:1154:G:OP2	2.38	0.57
52:D2:1009:A:N3	52:D2:1153:C:O2'	2.37	0.57
5:AE:86:ARG:NH2	51:D1:673:A:O3'	2.38	0.56
8:AH:24:ASN:OD1	8:AH:25:GLY:N	2.36	0.56
21:B0:51:ARG:NH2	52:D2:2364:C:OP1	2.35	0.56
28:B8:23:HIS:ND1	28:B8:24:LYS:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:BN:113:MET:HE3	39:BN:116:ILE:HD11	1.86	0.56
8:AH:104:THR:HG22	8:AH:106:ASP:H	1.70	0.56
11:AK:20:VAL:HG13	11:AK:94:TYR:CE1	2.40	0.56
34:BE:9:ASP:O	34:BE:13:LYS:NZ	2.39	0.56
40:BO:77:ILE:CG2	40:BO:110:VAL:HG22	2.34	0.56
45:BT:12:ARG:O	45:BT:16:ILE:HD12	2.06	0.56
48:BW:54:GLU:OE1	48:BW:54:GLU:N	2.36	0.56
52:D2:242:G:N2	52:D2:255:A:OP2	2.27	0.56
13:AM:12:ARG:NH2	51:D1:980:C:O3'	2.37	0.56
35:BF:105:SER:C	35:BF:106:LEU:HD12	2.31	0.56
39:BN:61:VAL:HG23	39:BN:87:LEU:HD11	1.88	0.56
43:BR:34:HIS:ND1	43:BR:53:THR:OG1	2.34	0.56
22:B1:41:SER:OG	22:B1:42:GLU:OE1	2.23	0.56
41:BP:44:ARG:NH1	52:D2:2484:G:OP1	2.35	0.56
48:BW:69:ARG:NH2	48:BW:72:GLN:OE1	2.38	0.56
50:BY:88:HIS:HE2	53:D3:75:G:HO2'	1.52	0.56
51:D1:427:U:O2'	51:D1:541:G:OP1	2.22	0.56
51:D1:664:G:H22	51:D1:741:G:H1	1.53	0.56
6:AF:41:ILE:HD11	51:D1:1240:U:O4'	2.06	0.56
45:BT:15:LYS:NZ	52:D2:1227:G:OP2	2.38	0.56
51:D1:811:C:O2'	51:D1:901:A:N1	2.39	0.56
4:AD:125:LYS:NZ	51:D1:9:G:OP2	2.30	0.56
6:AF:113:LYS:O	51:D1:1239:A:O2'	2.24	0.56
4:AD:152:VAL:HG11	7:AG:98:LEU:HD12	1.87	0.56
30:BA:30:LEU:HD12	30:BA:31:LYS:N	2.20	0.56
20:AT:66:ARG:NH2	51:D1:1099:G:OP1	2.37	0.56
31:BB:110:LYS:N	31:BB:113:ASP:OD2	2.37	0.56
32:BC:183:GLU:OE1	32:BC:183:GLU:N	2.36	0.56
34:BE:71:LYS:NZ	52:D2:2299:U:OP1	2.30	0.55
51:D1:208:U:O2'	51:D1:211:G:N1	2.35	0.55
51:D1:1346:A:O2'	51:D1:1348:U:O4'	2.21	0.55
33:BD:163:ASN:ND2	52:D2:320:A:N3	2.54	0.55
38:BM:88:THR:HG1	38:BM:91:GLU:CD	2.15	0.55
52:D2:476:G:N1	52:D2:479:A:OP2	2.38	0.55
17:AQ:14:ALA:HB3	17:AQ:47:ARG:CZ	2.36	0.55
33:BD:122:GLU:OE1	33:BD:122:GLU:N	2.38	0.55
51:D1:427:U:OP2	51:D1:428:G:O2'	2.08	0.55
1:AA:110:ILE:HD12	1:AA:151:LYS:HA	1.89	0.55
35:BF:41:GLU:OE2	35:BF:54:ARG:NE	2.38	0.55
41:BP:29:GLY:N	41:BP:104:GLU:OE1	2.39	0.55
51:D1:1181:G:O2'	51:D1:1182:G:N7	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:BM:39:LYS:NZ	52:D2:1009:A:OP1	2.39	0.55
7:AG:102:VAL:HG23	7:AG:125:ILE:HB	1.88	0.55
8:AH:54:VAL:HG11	8:AH:93:LEU:CD1	2.37	0.55
42:BQ:90:ARG:NH2	52:D2:2880:C:O3'	2.40	0.55
52:D2:792:A:N3	52:D2:2072:C:O2'	2.36	0.55
34:BE:133:GLU:CD	34:BE:135:ILE:HG22	2.32	0.55
37:BK:26:ALA:HB2	52:D2:1096:A:H2	1.71	0.55
52:D2:2532:G:N2	52:D2:2663:G:O2'	2.40	0.55
20:AT:15:LEU:HD23	20:AT:15:LEU:O	2.07	0.55
35:BF:102:ILE:HD11	35:BF:116:LEU:HD11	1.89	0.54
39:BN:38:ILE:HD13	39:BN:61:VAL:HG22	1.87	0.54
47:BV:36:LEU:CD2	47:BV:47:VAL:HG23	2.37	0.54
6:AF:24:LYS:NZ	51:D1:1375:A:OP1	2.39	0.54
7:AG:95:MET:HE3	7:AG:129:ALA:HB1	1.88	0.54
51:D1:575:G:O2'	51:D1:821:G:OP2	2.25	0.54
51:D1:1305:G:H22	51:D1:1331:G:H2'	1.72	0.54
9:AI:32:THR:O	9:AI:32:THR:HG23	2.07	0.54
52:D2:2104:C:N4	52:D2:2185:U:O4	2.40	0.54
2:AB:184:ASN:OD1	2:AB:185:THR:N	2.38	0.54
50:BY:88:HIS:NE2	53:D3:75:G:O2'	2.40	0.54
51:D1:1144:G:H21	51:D1:1146:A:H62	1.54	0.54
2:AB:30:ASP:OD1	2:AB:31:ASN:N	2.39	0.54
32:BC:11:MET:HG2	32:BC:25:THR:HG22	1.90	0.54
22:B1:22:ASN:OD1	52:D2:2079:U:O2'	2.26	0.54
44:BS:2:ASN:OD1	44:BS:3:ILE:N	2.41	0.54
51:D1:518:C:O2'	51:D1:530:G:N2	2.40	0.54
52:D2:1837:C:O2'	52:D2:1927:A:N3	2.37	0.54
7:AG:14:ARG:NH2	7:AG:74:ILE:O	2.41	0.54
52:D2:500:G:N1	52:D2:503:A:OP2	2.40	0.54
19:AS:27:MET:O	19:AS:31:ILE:HD12	2.07	0.54
37:BK:58:ILE:HD11	37:BK:66:PHE:HD2	1.72	0.54
1:AA:13:VAL:HG23	1:AA:212:TYR:OH	2.08	0.54
13:AM:44:VAL:O	13:AM:48:GLN:NE2	2.41	0.54
32:BC:156:PHE:CG	38:BM:81:ILE:HD11	2.43	0.54
52:D2:1730:C:O2	52:D2:1731:G:N1	2.41	0.54
52:D2:2063:C:O2'	55:D5:76:A:O2'	1.97	0.54
52:D2:2134:A:C5	52:D2:2156:G:N2	2.76	0.54
13:AM:23:ARG:NH2	13:AM:50:LEU:HD21	2.23	0.53
37:BK:4:VAL:HG22	37:BK:7:TYR:HE1	1.73	0.53
38:BM:95:ARG:NH2	52:D2:2640:G:OP2	2.41	0.53
47:BV:36:LEU:HD21	47:BV:47:VAL:HG23	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:D2:1791:A:N6	52:D2:1828:G:O2'	2.34	0.53
53:D3:14:U:OP2	53:D3:70:C:O2'	2.26	0.53
21:B0:67:VAL:HG12	21:B0:67:VAL:O	2.08	0.53
34:BE:68:LYS:NZ	53:D3:41:G:O6	2.27	0.53
2:AB:92:ASP:OD1	2:AB:93:ILE:N	2.41	0.53
52:D2:227:A:HO2'	52:D2:228:C:P	2.31	0.53
28:B8:27:ASN:O	28:B8:35:LYS:NZ	2.32	0.53
30:BA:205:LYS:NZ	52:D2:1860:G:OP1	2.39	0.53
52:D2:1085:A:O2'	52:D2:1086:A:O4'	2.23	0.53
5:AE:38:ARG:O	5:AE:39:LEU:HD22	2.09	0.53
14:AN:1:SER:OG	14:AN:34:GLN:NE2	2.42	0.53
28:B8:18:LYS:NZ	52:D2:652:U:OP2	2.40	0.53
27:B7:24:THR:HG23	27:B7:27:GLY:H	1.72	0.53
51:D1:167:A:N6	51:D1:168:G:O6	2.41	0.53
51:D1:976:G:OP2	51:D1:1358:U:O2'	2.27	0.53
51:D1:1196:A:O2'	51:D1:1197:A:OP2	2.21	0.53
52:D2:280:U:O4	52:D2:361:G:N2	2.42	0.53
37:BK:58:ILE:HD11	37:BK:66:PHE:CD2	2.44	0.53
3:AC:84:ASN:ND2	3:AC:87:GLU:OE1	2.41	0.53
52:D2:1093:G:H21	52:D2:1098:A:H62	1.56	0.53
32:BC:136:ASN:OD1	32:BC:137:SER:N	2.42	0.53
4:AD:149:PRO:HA	4:AD:152:VAL:HG12	1.90	0.52
41:BP:53:MET:HE3	41:BP:120:ALA:HB2	1.91	0.52
32:BC:51:THR:HB	32:BC:79:LEU:HD23	1.90	0.52
37:BK:104:GLN:HE22	37:BK:108:ILE:HD12	1.75	0.52
48:BW:11:LEU:HD13	48:BW:32:LEU:HD13	1.91	0.52
52:D2:1450:G:H21	52:D2:1452:G:H1	1.57	0.52
6:AF:14:ASP:OD2	6:AF:22:LEU:HD23	2.09	0.52
52:D2:532:A:N7	52:D2:2021:C:O2'	2.39	0.52
52:D2:886:A:H1'	52:D2:890:C:H41	1.74	0.52
52:D2:2473:U:OP1	52:D2:2529:G:N2	2.41	0.52
14:AN:31:LEU:HD22	14:AN:62:ARG:HB2	1.91	0.52
31:BB:227:VAL:HG13	31:BB:228:ASP:OD1	2.09	0.52
36:BI:135:HIS:ND1	36:BI:137:GLU:OE1	2.42	0.52
43:BR:25:ARG:NH2	53:D3:8:C:O3'	2.42	0.52
11:AK:20:VAL:HG13	11:AK:94:TYR:HE1	1.74	0.52
12:AL:51:GLN:N	12:AL:51:GLN:OE1	2.41	0.52
31:BB:50:THR:HG23	31:BB:53:ILE:HD12	1.92	0.52
2:AB:41:TYR:O	2:AB:44:LYS:N	2.43	0.52
17:AQ:21:ASP:OD1	17:AQ:22:TYR:N	2.43	0.52
52:D2:1026:G:OP2	52:D2:1134:A:O2'	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:D2:1490:A:O2'	52:D2:1491:G:OP1	2.27	0.52
12:AL:39:ALA:O	12:AL:42:VAL:HG22	2.08	0.52
30:BA:188:ASN:OD1	30:BA:189:LEU:N	2.42	0.52
51:D1:1495:U:O2'	52:D2:1919:A:N1	2.41	0.52
52:D2:1326:U:O2'	52:D2:2010:G:O2'	2.06	0.52
52:D2:1527:G:N1	52:D2:1544:A:OP2	2.38	0.52
18:AR:2:ARG:O	51:D1:1314:C:N4	2.43	0.52
49:BX:96:LYS:O	49:BX:97:SER:OG	2.26	0.52
3:AC:10:LEU:HD13	3:AC:62:ARG:HD2	1.93	0.51
4:AD:80:LEU:HD13	4:AD:122:VAL:HG11	1.92	0.51
45:BT:65:ASN:ND2	52:D2:1010:A:OP1	2.42	0.51
52:D2:1048:A:OP2	52:D2:1110:G:N2	2.42	0.51
8:AH:84:ARG:NH2	51:D1:1119:C:OP1	2.43	0.51
14:AN:57:ARG:NH1	14:AN:61:GLN:OE1	2.43	0.51
44:BS:83:ILE:HG22	44:BS:83:ILE:O	2.10	0.51
52:D2:2581:G:N2	52:D2:2581:G:OP2	2.42	0.51
44:BS:38:ARG:NH2	51:D1:346:G:OP1	2.43	0.51
47:BV:96:ILE:HG22	52:D2:2013:A:H4'	1.93	0.51
50:BY:45:ASP:OD1	50:BY:46:LYS:N	2.43	0.51
51:D1:324:G:N1	51:D1:327:A:OP2	2.44	0.51
52:D2:1900:A:HO2'	52:D2:1901:A:P	2.34	0.51
52:D2:2061:G:O2'	52:D2:2062:A:OP2	2.23	0.51
3:AC:94:GLU:OE2	3:AC:103:ARG:NH1	2.44	0.51
36:BI:80:ILE:HD11	36:BI:146:VAL:HG22	1.92	0.51
40:BO:95:LEU:O	40:BO:100:ILE:HG22	2.10	0.51
4:AD:123:LEU:HD12	4:AD:123:LEU:O	2.11	0.51
20:AT:39:LYS:NZ	51:D1:1530:G:O6	2.32	0.51
35:BF:72:ASN:O	35:BF:76:ILE:HD12	2.11	0.51
37:BK:23:VAL:CG1	37:BK:26:ALA:HB3	2.40	0.51
47:BV:24:ILE:HD13	47:BV:36:LEU:HD11	1.92	0.51
2:AB:153:SER:OG	2:AB:164:THR:HG22	2.11	0.51
4:AD:80:LEU:CD1	4:AD:122:VAL:HG11	2.40	0.51
7:AG:11:THR:HG21	51:D1:876:C:H1'	1.93	0.51
12:AL:2:ARG:O	12:AL:56:ARG:NH2	2.42	0.51
37:BK:26:ALA:HB2	52:D2:1096:A:C2	2.45	0.51
41:BP:47:GLU:OE2	41:BP:51:ARG:NH2	2.44	0.51
52:D2:2134:A:N6	52:D2:2156:G:C2	2.79	0.51
34:BE:161:SER:N	34:BE:164:GLU:OE2	2.43	0.51
35:BF:19:ASN:O	35:BF:22:VAL:HG12	2.10	0.51
38:BM:88:THR:OG1	38:BM:91:GLU:OE1	2.28	0.51
52:D2:2835:A:N6	52:D2:2879:A:OP2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B1:2:ARG:HD2	22:B1:29:LEU:HD12	1.93	0.51
36:BI:55:GLU:OE1	36:BI:55:GLU:N	2.42	0.51
47:BV:43:ALA:O	47:BV:47:VAL:HG22	2.11	0.51
30:BA:44:VAL:HG12	30:BA:214:ILE:HG22	1.93	0.50
34:BE:139:GLU:OE1	34:BE:139:GLU:N	2.44	0.50
38:BM:125:TYR:OH	38:BM:132:HIS:NE2	2.43	0.50
51:D1:157:U:O2	51:D1:164:G:O6	2.28	0.50
52:D2:704:G:H2'	52:D2:726:G:H22	1.76	0.50
52:D2:1857:G:O2'	52:D2:1885:A:N6	2.45	0.50
3:AC:13:ARG:NE	51:D1:543:U:OP1	2.43	0.50
40:BO:85:VAL:HG23	40:BO:86:GLU:H	1.76	0.50
51:D1:67:C:O2'	51:D1:171:A:O2'	2.07	0.50
52:D2:1712:U:OP2	52:D2:1713:A:O2'	2.26	0.50
4:AD:98:ALA:O	4:AD:101:GLY:N	2.44	0.50
34:BE:110:ILE:HG22	34:BE:136:ILE:HD13	1.92	0.50
37:BK:12:VAL:HG22	52:D2:1061:U:C2	2.47	0.50
42:BQ:1:MET:N	52:D2:1654:A:OP2	2.35	0.50
42:BQ:116:VAL:HG23	42:BQ:116:VAL:O	2.11	0.50
52:D2:1081:U:O4	52:D2:1082:U:O4	2.28	0.50
9:AI:14:ASP:OD1	9:AI:14:ASP:N	2.43	0.50
35:BF:31:GLU:C	35:BF:32:LEU:HD12	2.37	0.50
29:B9:36:ARG:NH1	52:D2:2742:G:OP1	2.44	0.50
45:BT:82:LEU:HD12	45:BT:112:ALA:HB2	1.93	0.50
51:D1:509:A:N3	51:D1:543:U:O2'	2.42	0.50
52:D2:2258:C:O2'	52:D2:2427:C:OP2	2.28	0.50
33:BD:119:ILE:HB	33:BD:187:VAL:HG12	1.93	0.50
52:D2:276:U:O2'	52:D2:278:A:N6	2.43	0.50
6:AF:5:VAL:O	6:AF:5:VAL:HG12	2.12	0.50
31:BB:164:VAL:HG12	31:BB:172:THR:O	2.12	0.50
41:BP:123:LYS:NZ	52:D2:2483:C:N3	2.57	0.50
5:AE:3:HIS:H	5:AE:92:THR:HG22	1.76	0.50
35:BF:106:LEU:HD23	35:BF:151:ARG:HG3	1.92	0.50
51:D1:421:U:O2'	51:D1:422:C:OP2	2.27	0.50
52:D2:624:C:O2'	52:D2:657:U:OP1	2.30	0.50
7:AG:103:VAL:HG22	7:AG:124:ILE:HD13	1.94	0.50
33:BD:148:ILE:HD13	33:BD:187:VAL:CG2	2.42	0.50
51:D1:1397:C:O2'	51:D1:1398:A:OP1	2.25	0.50
1:AA:156:LEU:HD12	1:AA:157:PRO:HD2	1.94	0.49
18:AR:11:ASP:OD2	18:AR:34:SER:OG	2.28	0.49
20:AT:11:PHE:O	20:AT:13:VAL:HG22	2.12	0.49
10:AJ:87:GLY:O	10:AJ:92:ARG:NE	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B3:3:THR:OG1	24:B3:36:GLU:OE2	2.20	0.49
47:BV:78:GLU:O	52:D2:24:G:O2'	2.30	0.49
51:D1:1301:U:O2'	51:D1:1302:C:OP1	2.23	0.49
52:D2:1236:G:O2'	52:D2:1237:A:O5'	2.26	0.49
6:AF:50:ALA:O	6:AF:54:GLY:N	2.43	0.49
34:BE:11:VAL:HG22	34:BE:15:LEU:HD23	1.94	0.49
35:BF:1:SER:OG	35:BF:2:ARG:N	2.45	0.49
27:B7:12:ARG:HD3	27:B7:44:VAL:HG21	1.94	0.49
34:BE:163:GLU:OE1	34:BE:166:ARG:NH2	2.44	0.49
52:D2:1930:G:HO2'	52:D2:1931:U:P	2.36	0.49
53:D3:30:C:H1'	53:D3:57:A:H61	1.76	0.49
3:AC:58:GLN:O	3:AC:62:ARG:HG2	2.12	0.49
16:AP:12:VAL:CG2	16:AP:21:VAL:HG13	2.42	0.49
34:BE:33:ILE:HD12	34:BE:95:MET:HG3	1.95	0.49
51:D1:1399:C:O2	51:D1:1502:A:N6	2.45	0.49
52:D2:550:C:N4	52:D2:551:G:O6	2.45	0.49
52:D2:948:C:O2	52:D2:984:A:O2'	2.21	0.49
52:D2:1173:U:O2'	52:D2:1177:G:N2	2.46	0.49
52:D2:1918:A:O2'	52:D2:1920:C:N4	2.46	0.49
9:AI:65:TYR:HB3	13:AM:95:LEU:HD11	1.95	0.49
21:B0:11:ASP:OD1	21:B0:12:SER:N	2.43	0.49
52:D2:1056:G:N1	52:D2:1102:C:OP2	2.40	0.49
7:AG:82:LEU:HD12	7:AG:82:LEU:O	2.13	0.49
10:AJ:17:ASP:OD1	10:AJ:17:ASP:N	2.43	0.49
11:AK:47:ALA:C	11:AK:48:LEU:HD22	2.38	0.49
17:AQ:61:ALA:HB1	17:AQ:67:LEU:HD23	1.93	0.49
10:AJ:111:ASP:OD1	10:AJ:113:THR:OG1	2.18	0.49
37:BK:23:VAL:HG12	37:BK:26:ALA:HB3	1.95	0.49
45:BT:69:ARG:NH2	52:D2:1012:U:OP2	2.45	0.49
46:BU:14:VAL:HG22	46:BU:98:ILE:HD13	1.95	0.49
2:AB:46:LEU:HD12	2:AB:46:LEU:O	2.13	0.49
4:AD:162:GLU:O	7:AG:113:ARG:NH1	2.46	0.49
16:AP:71:SER:O	16:AP:71:SER:OG	2.31	0.49
29:B9:36:ARG:HG3	29:B9:37:GLN:H	1.78	0.49
35:BF:66:THR:O	35:BF:70:LEU:HD23	2.12	0.49
35:BF:88:LEU:CB	35:BF:161:VAL:HG12	2.42	0.49
51:D1:993:G:H2'	51:D1:995:C:H41	1.77	0.49
52:D2:75:G:H22	52:D2:111:A:H2	1.61	0.49
52:D2:1283:G:N2	52:D2:1286:A:OP2	2.46	0.49
12:AL:48:SER:OG	12:AL:51:GLN:OE1	2.24	0.48
44:BS:30:TRP:NE1	44:BS:81:ASP:OD2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:D2:859:G:O2'	52:D2:860:U:P	2.71	0.48
55:D5:22:G:N7	55:D5:46:G:N2	2.49	0.48
8:AH:129:ARG:NH1	55:D5:33:U:OP2	2.43	0.48
35:BF:109:SER:OG	52:D2:2667:C:N3	2.44	0.48
38:BM:98:GLU:N	38:BM:98:GLU:OE1	2.45	0.48
1:AA:34:ARG:O	1:AA:37:VAL:HG22	2.13	0.48
40:BO:85:VAL:HG23	40:BO:86:GLU:N	2.29	0.48
49:BX:5:ARG:NH2	52:D2:84:A:OP1	2.41	0.48
5:AE:19:PRO:HA	5:AE:22:ILE:HG12	1.96	0.48
31:BB:141:HIS:ND1	31:BB:192:GLY:O	2.44	0.48
47:BV:42:LYS:O	47:BV:45:VAL:HG12	2.13	0.48
51:D1:977:A:O2'	51:D1:979:C:OP2	2.29	0.48
11:AK:23:LEU:HD23	11:AK:29:LYS:HD3	1.95	0.48
51:D1:662:U:O2'	51:D1:836:G:OP1	2.32	0.48
52:D2:1328:A:O2'	52:D2:1329:U:O5'	2.29	0.48
22:B1:36:ARG:NH1	52:D2:2200:C:OP2	2.47	0.48
31:BB:117:SER:OG	31:BB:118:GLY:N	2.46	0.48
44:BS:50:ARG:NH2	52:D2:2683:C:OP1	2.45	0.48
45:BT:93:ILE:HD13	46:BU:11:GLN:HB2	1.95	0.48
47:BV:22:ASP:OD2	47:BV:25:ARG:NH1	2.43	0.48
7:AG:11:THR:HG22	7:AG:14:ARG:HH12	1.79	0.48
34:BE:99:PHE:O	34:BE:103:ILE:HD12	2.13	0.48
7:AG:74:ILE:HG13	7:AG:128:VAL:HG12	1.96	0.48
7:AG:81:GLY:N	51:D1:878:A:OP1	2.44	0.48
8:AH:20:ILE:HG22	8:AH:62:LEU:HD13	1.95	0.48
10:AJ:126:ARG:O	20:AT:34:ARG:NH2	2.47	0.48
11:AK:49:ARG:NH2	51:D1:522:C:H41	2.12	0.48
19:AS:53:MET:SD	19:AS:57:VAL:HG21	2.54	0.48
34:BE:96:TRP:O	34:BE:100:GLU:OE1	2.32	0.48
34:BE:110:ILE:HD11	34:BE:113:PHE:HD1	1.78	0.48
37:BK:75:ALA:CB	37:BK:131:THR:HG21	2.43	0.48
52:D2:1730:C:O2'	52:D2:1731:G:O5'	2.28	0.48
35:BF:166:GLU:OE1	35:BF:166:GLU:N	2.41	0.48
52:D2:1059:G:C2	52:D2:1080:A:C2	3.02	0.48
5:AE:38:ARG:C	5:AE:39:LEU:HD22	2.38	0.48
18:AR:42:ASN:OD1	18:AR:43:MET:N	2.46	0.48
39:BN:104:THR:OG1	39:BN:106:GLU:OE1	2.26	0.48
51:D1:197:A:O2'	51:D1:220:G:N2	2.47	0.48
52:D2:2391:G:H2'	52:D2:2424:C:H41	1.79	0.48
14:AN:54:GLY:O	14:AN:58:MET:HE3	2.14	0.47
39:BN:70:ARG:HG2	39:BN:76:VAL:HG12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:D2:372:G:O2'	52:D2:373:U:OP2	2.29	0.47
7:AG:63:LYS:HB3	7:AG:70:VAL:HG21	1.96	0.47
12:AL:16:ILE:O	12:AL:19:THR:OG1	2.20	0.47
52:D2:1071:G:N3	52:D2:1089:A:O2'	2.45	0.47
22:B1:60:LYS:NZ	52:D2:372:G:O4'	2.41	0.47
31:BB:156:SER:O	31:BB:159:THR:HG22	2.14	0.47
41:BP:86:LYS:NZ	52:D2:955:U:OP1	2.41	0.47
43:BR:69:ASP:OD1	43:BR:70:ALA:N	2.47	0.47
52:D2:58:G:O2'	52:D2:73:A:N1	2.39	0.47
52:D2:2031:A:N3	52:D2:2455:G:O2'	2.45	0.47
21:B0:33:ILE:HG22	21:B0:34:VAL:HG23	1.96	0.47
23:B2:49:ASP:O	23:B2:53:VAL:HG23	2.14	0.47
22:B1:31:ASN:ND2	52:D2:2230:G:N3	2.62	0.47
25:B5:53:VAL:HG21	42:BQ:98:LEU:HD11	1.96	0.47
22:B1:13:THR:HG21	52:D2:189:G:OP2	2.14	0.47
30:BA:67:HIS:NE2	30:BA:187:GLU:OE2	2.46	0.47
1:AA:101:THR:N	1:AA:174:GLU:OE2	2.41	0.47
1:AA:207:ARG:O	1:AA:210:THR:OG1	2.26	0.47
6:AF:39:GLU:HA	6:AF:42:VAL:HG12	1.97	0.47
10:AJ:34:THR:OG1	10:AJ:39:ASN:N	2.48	0.47
11:AK:47:ALA:O	11:AK:48:LEU:HD22	2.15	0.47
17:AQ:66:LEU:C	17:AQ:67:LEU:HD22	2.40	0.47
31:BB:220:ARG:NH2	52:D2:1788:C:OP1	2.48	0.47
52:D2:1581:G:H2'	52:D2:1582:C:C6	2.49	0.47
52:D2:1730:C:HO2'	52:D2:1731:G:P	2.38	0.47
2:AB:39:ARG:NH1	2:AB:54:ILE:O	2.48	0.47
3:AC:17:ASP:OD1	3:AC:18:LEU:N	2.48	0.47
15:AO:55:ASP:OD1	15:AO:56:ARG:N	2.48	0.47
16:AP:10:ARG:NH1	16:AP:12:VAL:HG12	2.29	0.47
24:B3:19:HIS:O	24:B3:23:LEU:HD23	2.14	0.47
25:B5:28:SER:O	25:B5:37:HIS:N	2.38	0.47
30:BA:193:LEU:HD21	30:BA:212:VAL:HG11	1.96	0.47
16:AP:69:THR:HG22	16:AP:70:LYS:H	1.80	0.47
21:B0:50:GLY:N	21:B0:54:THR:O	2.46	0.47
38:BM:84:ILE:HD11	52:D2:1131:G:O4'	2.15	0.47
48:BW:57:VAL:HG12	48:BW:86:THR:CG2	2.45	0.47
51:D1:673:A:H2'	51:D1:674:G:C8	2.50	0.47
1:AA:103:TRP:HA	1:AA:106:VAL:HG22	1.97	0.47
13:AM:53:ASP:OD1	13:AM:58:ARG:NE	2.43	0.47
23:B2:47:ARG:O	23:B2:50:VAL:HG12	2.15	0.47
24:B3:40:THR:OG1	24:B3:41:PRO:HD2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B7:12:ARG:HH11	27:B7:44:VAL:HG21	1.80	0.47
34:BE:56:LEU:HA	34:BE:59:ILE:HG22	1.97	0.47
48:BW:57:VAL:HG22	48:BW:58:VAL:H	1.80	0.47
49:BX:80:ASP:OD1	49:BX:81:ARG:N	2.48	0.47
5:AE:4:TYR:CE2	5:AE:71:ILE:HG21	2.50	0.46
34:BE:23:SER:N	34:BE:26:GLN:OE1	2.43	0.46
38:BM:98:GLU:OE2	38:BM:126:ALA:N	2.48	0.46
39:BN:121:GLU:OE2	44:BS:65:ASN:ND2	2.48	0.46
52:D2:2638:G:HO2'	52:D2:2639:A:C5'	2.27	0.46
52:D2:2645:G:OP2	52:D2:2645:G:N2	2.37	0.46
8:AH:109:GLN:OE1	8:AH:109:GLN:N	2.47	0.46
51:D1:692:U:O2'	51:D1:694:A:N7	2.37	0.46
5:AE:3:HIS:N	5:AE:92:THR:HG22	2.30	0.46
32:BC:29:VAL:HB	32:BC:98:VAL:HG22	1.98	0.46
40:BO:143:GLU:N	40:BO:143:GLU:OE1	2.48	0.46
1:AA:123:GLY:O	1:AA:127:LYS:NZ	2.39	0.46
48:BW:27:SER:O	48:BW:29:THR:HG23	2.15	0.46
2:AB:155:ARG:NH1	51:D1:1055:A:N3	2.64	0.46
10:AJ:28:ASN:OD1	10:AJ:29:THR:N	2.45	0.46
11:AK:72:ASN:N	11:AK:72:ASN:OD1	2.48	0.46
40:BO:11:GLY:O	52:D2:597:G:O2'	2.33	0.46
51:D1:652:U:O4	51:D1:752:G:O2'	2.12	0.46
8:AH:113:LYS:NZ	51:D1:1367:C:OP2	2.46	0.46
13:AM:3:GLN:OE1	13:AM:3:GLN:N	2.44	0.46
33:BD:143:LEU:HB3	33:BD:146:VAL:HG11	1.98	0.46
51:D1:362:G:N2	51:D1:365:U:OP2	2.42	0.46
51:D1:1222:G:OP2	51:D1:1322:C:N4	2.39	0.46
52:D2:1223:G:N2	52:D2:1226:A:OP2	2.46	0.46
8:AH:68:GLY:O	8:AH:74:GLN:NE2	2.49	0.46
19:AS:34:VAL:HG22	19:AS:49:ALA:HB1	1.97	0.46
20:AT:18:PHE:O	20:AT:21:SER:OG	2.22	0.46
31:BB:44:ASN:N	52:D2:1812:U:O2'	2.46	0.46
51:D1:685:G:N1	51:D1:704:A:OP2	2.44	0.46
52:D2:463:G:N2	52:D2:466:A:OP2	2.36	0.46
4:AD:162:GLU:OE1	4:AD:162:GLU:N	2.40	0.46
46:BU:39:LEU:O	46:BU:49:ILE:HD13	2.16	0.46
4:AD:104:ILE:HD13	4:AD:121:ASN:O	2.16	0.46
16:AP:13:SER:O	16:AP:21:VAL:HG12	2.16	0.46
23:B2:41:HIS:ND1	52:D2:95:A:O2'	2.43	0.46
50:BY:77:VAL:HG12	50:BY:89:ILE:CD1	2.46	0.46
52:D2:1668:A:O2'	52:D2:1674:G:N7	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:35:ASP:HA	2:AB:38:VAL:HG22	1.97	0.46
34:BE:140:ILE:HD12	34:BE:145:VAL:HG11	1.98	0.46
4:AD:97:PRO:O	4:AD:122:VAL:HG12	2.15	0.45
6:AF:73:GLU:N	6:AF:73:GLU:OE1	2.49	0.45
9:AI:57:VAL:HG23	9:AI:57:VAL:O	2.17	0.45
11:AK:46:SER:OG	51:D1:519:C:OP2	2.35	0.45
11:AK:74:GLN:O	11:AK:74:GLN:HG2	2.16	0.45
30:BA:51:ASP:OD1	30:BA:52:ALA:N	2.48	0.45
32:BC:60:VAL:HG13	32:BC:60:VAL:O	2.16	0.45
51:D1:1268:G:N3	51:D1:1326:U:O2'	2.48	0.45
6:AF:71:THR:HG22	6:AF:141:HIS:CE1	2.51	0.45
9:AI:37:ARG:NH2	51:D1:1125:U:OP1	2.49	0.45
47:BV:24:ILE:HG21	47:BV:36:LEU:HD11	1.98	0.45
52:D2:265:A:N1	52:D2:427:U:O2'	2.48	0.45
31:BB:22:GLU:OE2	31:BB:80:LEU:HD12	2.17	0.45
52:D2:1941:C:N4	52:D2:1965:C:O4'	2.49	0.45
52:D2:2638:G:H1'	52:D2:2778:A:H61	1.82	0.45
12:AL:96:VAL:HG22	51:D1:1308:U:OP1	2.16	0.45
20:AT:23:GLU:HG3	20:AT:24:LYS:H	1.82	0.45
30:BA:16:ASP:OD2	30:BA:19:LYS:N	2.49	0.45
34:BE:7:TYR:HA	34:BE:11:VAL:HG12	1.98	0.45
52:D2:1779:U:OP2	52:D2:1784:A:N6	2.44	0.45
51:D1:1536:C:N4	51:D1:1537:U:O4	2.50	0.45
6:AF:34:LYS:NZ	51:D1:1290:G:OP1	2.40	0.45
33:BD:18:THR:O	33:BD:110:SER:OG	2.34	0.45
47:BV:61:ASN:ND2	52:D2:495:G:N3	2.64	0.45
51:D1:511:C:O2'	51:D1:512:U:O5'	2.23	0.45
52:D2:630:G:N2	52:D2:633:A:OP2	2.44	0.45
2:AB:91:ALA:O	2:AB:95:GLY:N	2.50	0.45
6:AF:112:ASP:OD1	6:AF:112:ASP:N	2.50	0.45
38:BM:37:ARG:NH1	52:D2:1007:C:OP1	2.49	0.45
52:D2:368:A:H2'	52:D2:369:U:O4'	2.17	0.45
3:AC:139:ASN:N	3:AC:181:PHE:O	2.50	0.45
8:AH:121:ARG:NH1	51:D1:1345:U:OP1	2.50	0.45
16:AP:67:SER:OG	51:D1:254:G:OP1	2.27	0.45
34:BE:161:SER:HG	34:BE:164:GLU:CD	2.22	0.45
37:BK:133:ARG:NH1	52:D2:1077:A:O3'	2.45	0.45
40:BO:128:THR:HG21	52:D2:637:A:OP2	2.17	0.45
41:BP:97:GLN:N	41:BP:97:GLN:OE1	2.50	0.45
47:BV:72:THR:HG21	47:BV:108:SER:HB3	1.99	0.45
2:AB:143:LEU:H	2:AB:143:LEU:HD23	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:D1:62:U:OP1	51:D1:385:C:O2'	2.35	0.44
31:BB:206:LYS:NZ	52:D2:729:G:OP2	2.45	0.44
32:BC:146:ILE:CD1	32:BC:155:VAL:HG11	2.44	0.44
32:BC:155:VAL:HG21	52:D2:2618:G:H21	1.82	0.44
35:BF:51:PHE:CE1	35:BF:71:LEU:HD22	2.52	0.44
9:AI:8:ILE:HD13	9:AI:100:ILE:HD13	1.99	0.44
10:AJ:107:THR:O	20:AT:6:ARG:NH1	2.50	0.44
46:BU:85:LYS:NZ	52:D2:1187:G:OP1	2.41	0.44
1:AA:110:ILE:HD13	1:AA:147:LEU:CD2	2.45	0.44
5:AE:5:GLU:HA	5:AE:63:ASN:HA	1.99	0.44
7:AG:14:ARG:NH1	51:D1:875:U:O2'	2.51	0.44
13:AM:24:ALA:O	13:AM:27:LYS:HG2	2.17	0.44
15:AO:74:LEU:O	15:AO:78:VAL:HG23	2.16	0.44
38:BM:96:ARG:NH1	52:D2:2639:A:O2'	2.49	0.44
46:BU:64:VAL:HG12	46:BU:95:ASP:O	2.17	0.44
47:BV:42:LYS:NZ	52:D2:2011:U:OP1	2.39	0.44
50:BY:9:ARG:NH1	53:D3:76:G:OP1	2.45	0.44
8:AH:45:MET:O	8:AH:48:ARG:N	2.50	0.44
23:B2:5:GLU:OE1	23:B2:5:GLU:N	2.51	0.44
31:BB:164:VAL:HG11	31:BB:180:MET:CE	2.47	0.44
51:D1:197:A:N1	51:D1:220:G:O2'	2.49	0.44
9:AI:92:LEU:HD23	9:AI:92:LEU:H	1.82	0.44
48:BW:34:VAL:HG21	48:BW:43:ILE:HD11	2.00	0.44
3:AC:150:LYS:HD2	3:AC:150:LYS:O	2.18	0.44
5:AE:18:VAL:N	5:AE:19:PRO:HD2	2.33	0.44
52:D2:774:G:HO2'	52:D2:775:G:P	2.41	0.44
4:AD:98:ALA:HB3	4:AD:122:VAL:HA	2.00	0.44
22:B1:31:ASN:OD1	22:B1:33:HIS:NE2	2.51	0.44
24:B3:39:ASP:OD2	24:B3:44:ARG:NH2	2.50	0.44
37:BK:12:VAL:HG22	52:D2:1061:U:N3	2.33	0.44
52:D2:2467:C:H2'	52:D2:2468:A:O4'	2.18	0.44
3:AC:8:LEU:HD13	3:AC:31:CYS:HB3	2.00	0.43
3:AC:154:VAL:O	3:AC:158:LEU:HD23	2.17	0.43
16:AP:49:ASN:OD1	16:AP:50:ASN:N	2.50	0.43
20:AT:11:PHE:O	20:AT:12:ASP:OD1	2.36	0.43
34:BE:70:ARG:NH1	52:D2:2298:A:OP1	2.43	0.43
45:BT:93:ILE:HD12	45:BT:93:ILE:H	1.82	0.43
10:AJ:112:VAL:HG12	10:AJ:112:VAL:O	2.17	0.43
11:AK:2:THR:O	11:AK:5:GLN:N	2.47	0.43
19:AS:24:ARG:NH2	51:D1:323:U:OP1	2.51	0.43
42:BQ:58:ASP:OD1	42:BQ:59:SER:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:D1:126:G:OP1	51:D1:605:U:O2'	2.26	0.43
9:AI:45:ARG:NH2	51:D1:1254:A:OP2	2.50	0.43
20:AT:39:LYS:N	20:AT:40:PRO:HD2	2.34	0.43
30:BA:37:LYS:NZ	52:D2:2128:G:OP2	2.49	0.43
52:D2:1068:G:H21	52:D2:1095:A:H1'	1.83	0.43
52:D2:1724:G:O6	52:D2:1737:G:N2	2.51	0.43
4:AD:101:GLY:O	4:AD:102:THR:OG1	2.34	0.43
7:AG:28:SER:OG	7:AG:56:PRO:O	2.31	0.43
32:BC:148:GLN:O	52:D2:2052:A:O2'	2.31	0.43
35:BF:23:ILE:HD13	35:BF:71:LEU:HD21	1.99	0.43
39:BN:44:LYS:O	39:BN:54:LYS:NZ	2.51	0.43
48:BW:40:LYS:CE	48:BW:60:THR:HG22	2.48	0.43
52:D2:242:G:O2'	52:D2:254:G:O6	2.36	0.43
26:B6:21:THR:CG2	28:B8:33:THR:HG22	2.48	0.43
30:BA:15:VAL:HG21	30:BA:220:ALA:HB3	2.00	0.43
32:BC:197:THR:O	52:D2:2820:A:N6	2.52	0.43
38:BM:60:ASP:OD1	38:BM:60:ASP:N	2.48	0.43
48:BW:29:THR:HG22	48:BW:86:THR:CB	2.49	0.43
48:BW:40:LYS:HE3	48:BW:60:THR:HG22	2.00	0.43
51:D1:1346:A:HO2'	51:D1:1348:U:C1'	2.30	0.43
52:D2:629:G:N3	52:D2:639:U:O2'	2.52	0.43
4:AD:48:GLY:N	4:AD:66:ALA:HB2	2.34	0.43
31:BB:79:ARG:NE	31:BB:81:GLU:OE2	2.32	0.43
31:BB:132:ARG:NH1	31:BB:186:ASP:OD1	2.49	0.43
46:BU:91:GLN:NE2	52:D2:993:G:N3	2.66	0.43
48:BW:29:THR:HG22	48:BW:86:THR:HB	1.99	0.43
51:D1:50:A:O2'	51:D1:360:G:N2	2.51	0.43
52:D2:2126:A:H2'	52:D2:2162:G:H21	1.82	0.43
1:AA:91:VAL:HG22	1:AA:150:ILE:HD11	2.00	0.43
1:AA:187:ASP:OD1	1:AA:188:THR:N	2.47	0.43
50:BY:77:VAL:HG12	50:BY:89:ILE:HD12	2.00	0.43
51:D1:130:A:N3	51:D1:263:A:O2'	2.38	0.43
52:D2:61:C:H2'	52:D2:62:U:O4'	2.19	0.43
52:D2:2134:A:H1'	52:D2:2159:G:H21	1.83	0.43
42:BQ:114:GLU:OE1	42:BQ:118:ARG:NH2	2.52	0.43
48:BW:3:ARG:O	48:BW:7:LEU:HD13	2.19	0.43
29:B9:36:ARG:HG3	29:B9:37:GLN:N	2.34	0.43
45:BT:5:ARG:NH1	52:D2:1251:C:OP2	2.52	0.43
48:BW:57:VAL:HG22	48:BW:58:VAL:N	2.34	0.43
50:BY:72:VAL:HG21	50:BY:91:PHE:HB3	2.01	0.43
51:D1:481:G:O2'	51:D1:483:C:N4	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:D2:614:A:OP1	52:D2:616:A:N6	2.51	0.43
1:AA:101:THR:HG23	1:AA:174:GLU:HG3	2.01	0.43
6:AF:47:GLU:O	6:AF:51:GLN:OE1	2.36	0.43
30:BA:21:TYR:HD2	30:BA:222:VAL:HG13	1.84	0.43
52:D2:421:C:HO2'	52:D2:422:A:P	2.41	0.43
42:BQ:106:ASP:N	42:BQ:106:ASP:OD1	2.49	0.42
52:D2:298:G:O2'	52:D2:322:A:N1	2.50	0.42
13:AM:62:ARG:NH2	51:D1:982:U:OP2	2.48	0.42
32:BC:83:ARG:NH1	52:D2:2637:U:OP1	2.47	0.42
51:D1:1048:G:O6	51:D1:1210:C:N4	2.52	0.42
52:D2:2822:G:O2'	52:D2:2824:C:OP2	2.31	0.42
5:AE:9:MET:HE3	5:AE:59:TYR:CE2	2.54	0.42
51:D1:187:G:N2	51:D1:190:A:OP2	2.50	0.42
3:AC:115:GLN:NE2	51:D1:407:U:O4'	2.52	0.42
7:AG:10:LEU:HD22	7:AG:74:ILE:HD11	2.01	0.42
9:AI:90:LEU:O	9:AI:92:LEU:HD23	2.19	0.42
13:AM:30:ILE:HG22	13:AM:30:ILE:O	2.20	0.42
16:AP:78:VAL:HG23	16:AP:79:GLU:OE1	2.20	0.42
34:BE:59:ILE:HG23	34:BE:60:SER:N	2.35	0.42
52:D2:458:G:O2'	52:D2:459:U:P	2.77	0.42
52:D2:2637:U:H2'	52:D2:2638:G:O4'	2.19	0.42
6:AF:79:VAL:HG12	6:AF:79:VAL:O	2.19	0.42
22:B1:58:ILE:HD11	22:B1:63:ILE:CD1	2.49	0.42
38:BM:10:THR:O	38:BM:10:THR:HG22	2.19	0.42
52:D2:2124:G:N2	52:D2:2175:C:O2	2.52	0.42
1:AA:4:SER:O	1:AA:8:MET:HE3	2.19	0.42
22:B1:38:TRP:NE1	22:B1:40:GLU:OE1	2.48	0.42
31:BB:16:VAL:HB	31:BB:203:VAL:HG22	2.01	0.42
46:BU:14:VAL:CG2	46:BU:98:ILE:HD13	2.49	0.42
48:BW:55:VAL:HG22	48:BW:87:LEU:HD23	2.01	0.42
50:BY:32:GLY:O	50:BY:93:ARG:NH1	2.52	0.42
51:D1:766:A:OP2	51:D1:812:G:N2	2.51	0.42
52:D2:366:C:N4	52:D2:367:G:O6	2.52	0.42
14:AN:31:LEU:HD23	14:AN:31:LEU:C	2.45	0.42
16:AP:39:ARG:NH1	51:D1:280:C:O2'	2.53	0.42
35:BF:91:VAL:HG13	35:BF:91:VAL:O	2.20	0.42
41:BP:26:VAL:O	41:BP:26:VAL:HG13	2.18	0.42
42:BQ:97:ILE:O	42:BQ:98:LEU:HD23	2.19	0.42
52:D2:1061:U:O2'	52:D2:1062:G:OP1	2.37	0.42
6:AF:58:LEU:H	6:AF:58:LEU:HD23	1.85	0.42
9:AI:43:PRO:HB3	51:D1:1150:A:H4'	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:BM:5:THR:HG21	52:D2:537:G:H5'	2.02	0.42
46:BU:14:VAL:HG23	46:BU:18:GLN:NE2	2.34	0.42
52:D2:1363:C:O2'	52:D2:1809:A:N3	2.47	0.42
33:BD:146:VAL:HG12	33:BD:185:LYS:HB2	2.02	0.42
52:D2:1900:A:O2'	52:D2:1901:A:P	2.77	0.42
9:AI:97:ASP:OD1	9:AI:98:VAL:N	2.53	0.42
47:BV:17:VAL:HG12	47:BV:76:VAL:HG21	2.02	0.42
52:D2:1019:U:OP1	52:D2:1035:U:O2'	2.26	0.42
52:D2:1141:U:H4'	52:D2:1142:A:O4'	2.20	0.42
8:AH:90:ASP:O	8:AH:92:SER:N	2.53	0.41
52:D2:1433:A:H2'	52:D2:1434:A:C8	2.54	0.41
52:D2:2140:G:N1	52:D2:2152:G:N7	2.68	0.41
9:AI:11:LYS:HB3	9:AI:71:LEU:HB3	2.02	0.41
13:AM:91:GLU:OE1	13:AM:91:GLU:N	2.54	0.41
42:BQ:63:ARG:NH2	52:D2:1454:C:O5'	2.53	0.41
51:D1:1009:U:C2	51:D1:1020:G:O6	2.73	0.41
51:D1:1446:A:O2'	51:D1:1447:A:O4'	2.33	0.41
9:AI:52:LEU:HD21	9:AI:59:LYS:HD2	2.03	0.41
13:AM:30:ILE:HG21	13:AM:43:ALA:CB	2.50	0.41
20:AT:36:PHE:O	20:AT:37:TYR:HB3	2.19	0.41
32:BC:197:THR:OG1	52:D2:2820:A:N1	2.53	0.41
37:BK:14:ALA:O	37:BK:50:LYS:NZ	2.50	0.41
41:BP:53:MET:SD	41:BP:116:ALA:HB1	2.60	0.41
52:D2:285:G:C6	52:D2:356:G:C6	3.08	0.41
52:D2:962:G:H21	52:D2:2250:G:H1	1.68	0.41
1:AA:40:ILE:HG21	1:AA:200:PRO:HB2	2.01	0.41
1:AA:134:LEU:HD22	1:AA:138:ARG:HH12	1.85	0.41
10:AJ:27:ASN:ND2	51:D1:692:U:OP2	2.48	0.41
15:AO:79:ASN:O	15:AO:81:ALA:N	2.50	0.41
21:B0:15:LYS:HB2	21:B0:17:LEU:HD13	2.01	0.41
22:B1:53:LYS:HE3	52:D2:372:G:O2'	2.19	0.41
36:BI:55:GLU:HA	36:BI:58:LEU:HB3	2.02	0.41
40:BO:101:ILE:HG13	40:BO:102:GLY:N	2.35	0.41
47:BV:24:ILE:HG21	47:BV:36:LEU:CD1	2.50	0.41
52:D2:1372:U:O2'	52:D2:2212:A:N3	2.44	0.41
2:AB:41:TYR:O	2:AB:45:GLU:OE1	2.39	0.41
8:AH:3:ASN:OD1	8:AH:4:GLN:N	2.54	0.41
16:AP:12:VAL:HG23	16:AP:21:VAL:HG13	2.01	0.41
17:AQ:32:ILE:HD11	17:AQ:36:GLY:O	2.20	0.41
33:BD:51:GLU:OE1	33:BD:51:GLU:N	2.54	0.41
42:BQ:12:ARG:O	42:BQ:17:ARG:NH1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:BS:113:LEU:HD12	44:BS:113:LEU:O	2.21	0.41
49:BX:32:LYS:HB3	49:BX:63:ALA:HB1	2.03	0.41
1:AA:49:PHE:HA	1:AA:199:ILE:HD12	2.02	0.41
7:AG:35:ILE:HA	7:AG:38:VAL:HG12	2.02	0.41
17:AQ:14:ALA:HB3	17:AQ:47:ARG:NH1	2.35	0.41
24:B3:7:THR:HG23	24:B3:55:LYS:HG2	2.02	0.41
35:BF:138:GLN:NE2	52:D2:2745:C:O2	2.44	0.41
52:D2:160:A:N7	52:D2:166:U:O4	2.53	0.41
1:AA:100:LEU:N	1:AA:174:GLU:OE2	2.47	0.41
3:AC:190:LEU:HD12	3:AC:192:ALA:H	1.85	0.41
4:AD:75:LEU:HD22	4:AD:119:VAL:HG12	2.02	0.41
7:AG:92:PRO:O	7:AG:116:ARG:NH2	2.45	0.41
34:BE:131:VAL:HG12	34:BE:151:LEU:HB2	2.03	0.41
34:BE:160:LYS:N	34:BE:164:GLU:OE2	2.53	0.41
51:D1:499:A:O4'	51:D1:547:A:N6	2.53	0.41
51:D1:1095:U:OP1	51:D1:1108:G:N2	2.47	0.41
53:D3:3:C:O2'	53:D3:4:C:OP1	2.34	0.41
13:AM:81:ILE:HD12	51:D1:1202:U:C2	2.56	0.41
16:AP:16:MET:HG2	16:AP:16:MET:O	2.21	0.41
31:BB:143:VAL:HB	31:BB:153:LEU:HB2	2.02	0.41
32:BC:118:PHE:O	52:D2:1654:A:O2'	2.37	0.41
34:BE:120:SER:OG	34:BE:128:SER:O	2.33	0.41
39:BN:113:MET:SD	39:BN:113:MET:N	2.94	0.41
51:D1:191:G:O6	51:D1:192:A:N6	2.54	0.41
52:D2:548:G:H2'	52:D2:549:G:O4'	2.20	0.41
1:AA:8:MET:CE	1:AA:46:VAL:HG22	2.51	0.41
6:AF:35:LYS:O	6:AF:39:GLU:OE1	2.39	0.41
6:AF:78:ARG:HB3	6:AF:83:THR:HA	2.02	0.41
7:AG:15:ASN:ND2	51:D1:826:C:O2	2.53	0.41
35:BF:93:TYR:OH	35:BF:159:LYS:NZ	2.26	0.41
39:BN:61:VAL:HG23	39:BN:87:LEU:HD13	2.02	0.41
44:BS:64:SER:OG	44:BS:65:ASN:OD1	2.37	0.41
53:D3:88:C:H4'	53:D3:89:U:OP1	2.21	0.41
2:AB:107:LYS:HD2	2:AB:107:LYS:O	2.20	0.41
3:AC:195:ASN:OD1	3:AC:197:HIS:ND1	2.53	0.41
5:AE:32:ALA:HB1	5:AE:70:VAL:HG11	2.03	0.41
22:B1:63:ILE:O	22:B1:67:LEU:HD23	2.21	0.41
33:BD:2:GLU:C	33:BD:3:LEU:HD22	2.45	0.41
33:BD:176:ASP:OD1	33:BD:179:SER:OG	2.36	0.41
39:BN:104:THR:HA	39:BN:122:VAL:HG11	2.02	0.41
47:BV:70:LYS:N	47:BV:108:SER:O	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:BY:47:VAL:HA	50:BY:50:MET:HE2	2.02	0.41
52:D2:1093:G:N2	52:D2:1098:A:H62	2.19	0.41
52:D2:2286:G:H21	52:D2:2287:A:N6	2.19	0.41
7:AG:74:ILE:O	7:AG:74:ILE:HG23	2.21	0.40
9:AI:44:THR:HG22	51:D1:1151:A:H5''	2.04	0.40
9:AI:74:VAL:O	9:AI:75:ASP:OD1	2.39	0.40
31:BB:131:MET:HE3	31:BB:143:VAL:HG13	2.03	0.40
32:BC:57:ALA:O	32:BC:60:VAL:HG12	2.20	0.40
36:BI:3:VAL:HG22	36:BI:36:ALA:HB1	2.03	0.40
40:BO:100:ILE:HG23	40:BO:101:ILE:HG23	2.03	0.40
47:BV:93:ALA:HB2	52:D2:1614:A:C2	2.56	0.40
52:D2:1024:G:HO2'	52:D2:1144:A:HO2'	1.67	0.40
52:D2:2266:A:H4'	52:D2:2267:A:N3	2.36	0.40
55:D5:21:A:H61	55:D5:46:G:H2'	1.86	0.40
1:AA:156:LEU:HD11	1:AA:180:ILE:HD11	2.03	0.40
5:AE:88:MET:HG2	5:AE:89:VAL:N	2.37	0.40
8:AH:29:ILE:HG21	8:AH:37:TYR:CD2	2.56	0.40
15:AO:36:VAL:O	15:AO:36:VAL:HG23	2.21	0.40
30:BA:217:THR:HB	52:D2:2124:G:H21	1.86	0.40
36:BI:11:ASN:C	36:BI:12:LEU:HD22	2.46	0.40
50:BY:75:GLN:HB2	50:BY:92:VAL:HG23	2.02	0.40
51:D1:578:C:O2'	51:D1:728:A:N3	2.46	0.40
52:D2:161:A:H3'	52:D2:162:U:H5''	2.03	0.40
52:D2:1716:U:OP2	52:D2:1743:G:N1	2.48	0.40
12:AL:99:GLN:OE1	12:AL:99:GLN:N	2.54	0.40
18:AR:39:ILE:HD12	18:AR:68:HIS:O	2.22	0.40
32:BC:40:LEU:HD13	32:BC:44:GLY:O	2.22	0.40
42:BQ:27:SER:OG	52:D2:1278:C:O2'	2.28	0.40
44:BS:46:VAL:HG22	44:BS:60:VAL:HG22	2.03	0.40
52:D2:421:C:O2'	52:D2:422:A:P	2.80	0.40
52:D2:1328:A:HO2'	52:D2:1329:U:P	2.43	0.40
52:D2:1697:G:OP2	52:D2:1698:A:O2'	2.33	0.40
3:AC:98:ASP:OD2	3:AC:99:ASN:N	2.54	0.40
4:AD:24:VAL:HG22	4:AD:25:LYS:H	1.86	0.40
8:AH:45:MET:SD	8:AH:45:MET:N	2.95	0.40
15:AO:6:LEU:HD22	15:AO:17:TYR:HB3	2.03	0.40
18:AR:24:SER:O	18:AR:27:LYS:NZ	2.54	0.40
31:BB:173:LEU:HD11	31:BB:183:VAL:HG12	2.04	0.40
32:BC:35:THR:HG21	32:BC:79:LEU:HD22	2.04	0.40
32:BC:164:GLN:NE2	52:D2:2822:G:OP1	2.47	0.40
32:BC:188:LEU:HD11	44:BS:7:LEU:HD11	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:BI:121:VAL:HG22	36:BI:121:VAL:O	2.22	0.40
37:BK:90:GLY:O	37:BK:91:LYS:CE	2.69	0.40
44:BS:114:ASN:OD1	44:BS:114:ASN:N	2.54	0.40
45:BT:86:SER:OG	45:BT:86:SER:O	2.39	0.40
47:BV:108:SER:OG	47:BV:109:ASP:N	2.54	0.40
52:D2:2627:G:O2'	52:D2:2781:A:N1	2.51	0.40
3:AC:11:SER:HA	3:AC:18:LEU:HD23	2.04	0.40
4:AD:132:PRO:HA	4:AD:135:VAL:HG22	2.02	0.40
5:AE:92:THR:OG1	5:AE:93:LYS:N	2.55	0.40
16:AP:59:GLU:OE1	16:AP:76:ARG:NE	2.55	0.40
30:BA:22:ASP:OD1	30:BA:23:ILE:N	2.54	0.40
41:BP:50:ARG:NH1	41:BP:54:THR:HG21	2.36	0.40
48:BW:58:VAL:HG13	48:BW:85:VAL:HG12	2.03	0.40
52:D2:1075:C:H2'	52:D2:1076:C:C6	2.56	0.40
52:D2:1508:A:H2'	52:D2:1509:A:O4'	2.21	0.40
52:D2:1779:U:O2	52:D2:1783:A:N6	2.54	0.40
52:D2:2100:G:O6	52:D2:2189:U:O4	2.39	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	223/241 (92%)	209 (94%)	14 (6%)	0	100	100
2	AB	204/233 (88%)	196 (96%)	8 (4%)	0	100	100
3	AC	203/206 (98%)	180 (89%)	23 (11%)	0	100	100
4	AD	155/167 (93%)	132 (85%)	22 (14%)	1 (1%)	21	51
5	AE	98/135 (73%)	81 (83%)	17 (17%)	0	100	100
6	AF	149/179 (83%)	138 (93%)	11 (7%)	0	100	100
7	AG	127/130 (98%)	120 (94%)	7 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	AH	125/130 (96%)	106 (85%)	19 (15%)	0	100	100
9	AI	96/103 (93%)	75 (78%)	21 (22%)	0	100	100
10	AJ	114/129 (88%)	96 (84%)	18 (16%)	0	100	100
11	AK	121/124 (98%)	100 (83%)	21 (17%)	0	100	100
12	AL	112/118 (95%)	101 (90%)	11 (10%)	0	100	100
13	AM	98/101 (97%)	82 (84%)	16 (16%)	0	100	100
14	AN	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	10	34
15	AO	80/82 (98%)	73 (91%)	7 (9%)	0	100	100
16	AP	78/84 (93%)	68 (87%)	10 (13%)	0	100	100
17	AQ	63/75 (84%)	59 (94%)	4 (6%)	0	100	100
18	AR	77/92 (84%)	70 (91%)	7 (9%)	0	100	100
19	AS	83/87 (95%)	77 (93%)	6 (7%)	0	100	100
20	AT	63/71 (89%)	45 (71%)	16 (25%)	2 (3%)	3	13
21	B0	73/85 (86%)	72 (99%)	1 (1%)	0	100	100
22	B1	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
23	B2	61/63 (97%)	58 (95%)	3 (5%)	0	100	100
24	B3	56/59 (95%)	52 (93%)	4 (7%)	0	100	100
25	B5	54/57 (95%)	49 (91%)	5 (9%)	0	100	100
26	B6	48/55 (87%)	46 (96%)	2 (4%)	0	100	100
27	B7	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
28	B8	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
29	B9	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
30	BA	130/234 (56%)	117 (90%)	13 (10%)	0	100	100
31	BB	269/273 (98%)	251 (93%)	18 (7%)	0	100	100
32	BC	207/209 (99%)	192 (93%)	15 (7%)	0	100	100
33	BD	199/201 (99%)	183 (92%)	15 (8%)	1 (0%)	24	54
34	BE	175/179 (98%)	157 (90%)	18 (10%)	0	100	100
35	BF	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
36	BI	147/149 (99%)	133 (90%)	14 (10%)	0	100	100
37	BK	139/142 (98%)	121 (87%)	18 (13%)	0	100	100
38	BM	140/142 (99%)	134 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	BN	120/123 (98%)	108 (90%)	12 (10%)	0	100	100
40	BO	141/144 (98%)	124 (88%)	17 (12%)	0	100	100
41	BP	134/136 (98%)	124 (92%)	10 (8%)	0	100	100
42	BQ	118/127 (93%)	107 (91%)	11 (9%)	0	100	100
43	BR	114/117 (97%)	111 (97%)	2 (2%)	1 (1%)	14	41
44	BS	112/115 (97%)	107 (96%)	5 (4%)	0	100	100
45	BT	115/118 (98%)	111 (96%)	4 (4%)	0	100	100
46	BU	101/103 (98%)	93 (92%)	7 (7%)	1 (1%)	12	39
47	BV	108/110 (98%)	98 (91%)	10 (9%)	0	100	100
48	BW	91/100 (91%)	86 (94%)	5 (6%)	0	100	100
49	BX	100/104 (96%)	93 (93%)	7 (7%)	0	100	100
50	BY	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
All	All	5790/6219 (93%)	5274 (91%)	509 (9%)	7 (0%)	49	77

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	AD	122	VAL
43	BR	34	HIS
46	BU	54	VAL
20	AT	36	PHE
14	AN	45	HIS
33	BD	83	VAL
20	AT	12	ASP

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AA	186/199 (94%)	186 (100%)	0	100	100
2	AB	170/190 (90%)	170 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	AC	172/173 (99%)	172 (100%)	0	100	100
4	AD	119/126 (94%)	119 (100%)	0	100	100
5	AE	87/116 (75%)	87 (100%)	0	100	100
6	AF	124/147 (84%)	124 (100%)	0	100	100
7	AG	104/105 (99%)	104 (100%)	0	100	100
8	AH	105/107 (98%)	105 (100%)	0	100	100
9	AI	86/90 (96%)	86 (100%)	0	100	100
10	AJ	89/99 (90%)	89 (100%)	0	100	100
11	AK	103/104 (99%)	103 (100%)	0	100	100
12	AL	92/96 (96%)	92 (100%)	0	100	100
13	AM	83/84 (99%)	83 (100%)	0	100	100
14	AN	76/77 (99%)	76 (100%)	0	100	100
15	AO	65/65 (100%)	65 (100%)	0	100	100
16	AP	74/78 (95%)	74 (100%)	0	100	100
17	AQ	56/65 (86%)	56 (100%)	0	100	100
18	AR	70/79 (89%)	70 (100%)	0	100	100
19	AS	65/66 (98%)	65 (100%)	0	100	100
20	AT	55/61 (90%)	55 (100%)	0	100	100
21	B0	57/63 (90%)	57 (100%)	0	100	100
22	B1	67/68 (98%)	67 (100%)	0	100	100
23	B2	55/55 (100%)	55 (100%)	0	100	100
24	B3	48/49 (98%)	48 (100%)	0	100	100
25	B5	47/48 (98%)	47 (100%)	0	100	100
26	B6	45/49 (92%)	45 (100%)	0	100	100
27	B7	38/38 (100%)	38 (100%)	0	100	100
28	B8	51/52 (98%)	51 (100%)	0	100	100
29	B9	34/34 (100%)	34 (100%)	0	100	100
30	BA	110/181 (61%)	110 (100%)	0	100	100
31	BB	216/218 (99%)	216 (100%)	0	100	100
32	BC	164/164 (100%)	164 (100%)	0	100	100
33	BD	165/165 (100%)	165 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	BE	148/150 (99%)	148 (100%)	0	100	100
35	BF	137/138 (99%)	137 (100%)	0	100	100
36	BI	114/114 (100%)	114 (100%)	0	100	100
37	BK	109/110 (99%)	109 (100%)	0	100	100
38	BM	116/116 (100%)	116 (100%)	0	100	100
39	BN	103/104 (99%)	103 (100%)	0	100	100
40	BO	102/103 (99%)	102 (100%)	0	100	100
41	BP	109/109 (100%)	109 (100%)	0	100	100
42	BQ	100/103 (97%)	100 (100%)	0	100	100
43	BR	86/87 (99%)	86 (100%)	0	100	100
44	BS	99/100 (99%)	99 (100%)	0	100	100
45	BT	89/90 (99%)	89 (100%)	0	100	100
46	BU	84/84 (100%)	84 (100%)	0	100	100
47	BV	93/93 (100%)	93 (100%)	0	100	100
48	BW	80/84 (95%)	80 (100%)	0	100	100
49	BX	83/85 (98%)	83 (100%)	0	100	100
50	BY	78/78 (100%)	78 (100%)	0	100	100
All	All	4808/5059 (95%)	4808 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
2	AB	99	GLN
2	AB	138	GLN
3	AC	125	ASN
3	AC	135	GLN
4	AD	88	HIS
4	AD	120	HIS
6	AF	67	ASN
7	AG	66	GLN
10	AJ	100	ASN
14	AN	19	ASN
30	BA	203	GLN
31	BB	133	ASN

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Mol	Chain	Res	Type
31	BB	259	ASN
35	BF	19	ASN
35	BF	21	GLN
35	BF	127	GLN
36	BI	33	GLN
37	BK	18	ASN
37	BK	104	GLN
38	BM	77	HIS
38	BM	136	GLN
39	BN	29	HIS
40	BO	38	GLN
44	BS	55	HIS
45	BT	51	GLN
50	BY	49	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
51	D1	1538/1540 (99%)	227 (14%)	9 (0%)
52	D2	2902/2903 (99%)	478 (16%)	25 (0%)
53	D3	119/120 (99%)	19 (15%)	1 (0%)
54	D4	6/56 (10%)	1 (16%)	0
55	D5	76/78 (97%)	9 (11%)	0
All	All	4641/4697 (98%)	734 (15%)	35 (0%)

All (734) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
51	D1	4	U
51	D1	6	G
51	D1	9	G
51	D1	31	G
51	D1	32	A
51	D1	39	G
51	D1	47	C
51	D1	48	C
51	D1	51	A
51	D1	71	A
51	D1	81	A
51	D1	82	G
51	D1	85	U

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Mol	Chain	Res	Type
51	D1	86	G
51	D1	87	C
51	D1	94	G
51	D1	95	C
51	D1	96	U
51	D1	100	G
51	D1	121	U
51	D1	130	A
51	D1	154	U
51	D1	164	G
51	D1	173	U
51	D1	181	A
51	D1	183	C
51	D1	184	G
51	D1	197	A
51	D1	209	U
51	D1	210	C
51	D1	211	G
51	D1	212	G
51	D1	245	U
51	D1	247	G
51	D1	251	G
51	D1	266	G
51	D1	267	C
51	D1	279	A
51	D1	280	C
51	D1	281	G
51	D1	283	U
51	D1	289	G
51	D1	306	A
51	D1	316	C
51	D1	328	C
51	D1	329	A
51	D1	347	G
51	D1	352	C
51	D1	354	G
51	D1	355	C
51	D1	367	U
51	D1	372	C
51	D1	373	A
51	D1	406	G
51	D1	411	A

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Mol	Chain	Res	Type
51	D1	412	A
51	D1	413	G
51	D1	422	C
51	D1	423	G
51	D1	424	G
51	D1	429	U
51	D1	438	U
51	D1	464	U
51	D1	467	U
51	D1	468	A
51	D1	474	G
51	D1	484	G
51	D1	486	U
51	D1	495	A
51	D1	496	A
51	D1	497	G
51	D1	509	A
51	D1	510	A
51	D1	511	C
51	D1	517	G
51	D1	518	C
51	D1	521	G
51	D1	527	G
51	D1	531	U
51	D1	532	A
51	D1	547	A
51	D1	559	A
51	D1	561	U
51	D1	564	C
51	D1	572	A
51	D1	573	A
51	D1	575	G
51	D1	576	C
51	D1	577	G
51	D1	596	A
51	D1	628	G
51	D1	653	U
51	D1	654	G
51	D1	665	A
51	D1	687	A
51	D1	688	G
51	D1	703	G

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Mol	Chain	Res	Type
51	D1	704	A
51	D1	718	A
51	D1	723	U
51	D1	724	G
51	D1	731	G
51	D1	733	G
51	D1	754	C
51	D1	755	G
51	D1	777	A
51	D1	794	A
51	D1	803	G
51	D1	815	A
51	D1	817	C
51	D1	818	G
51	D1	819	A
51	D1	832	G
51	D1	842	U
51	D1	843	U
51	D1	844	G
51	D1	845	A
51	D1	846	G
51	D1	851	G
51	D1	872	A
51	D1	890	G
51	D1	891	U
51	D1	902	G
51	D1	914	A
51	D1	920	U
51	D1	934	C
51	D1	935	A
51	D1	960	U
51	D1	961	U
51	D1	966	G
51	D1	969	A
51	D1	971	G
51	D1	975	A
51	D1	976	G
51	D1	977	A
51	D1	992	U
51	D1	993	G
51	D1	994	A
51	D1	1004	A

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Mol	Chain	Res	Type
51	D1	1020	G
51	D1	1022	A
51	D1	1026	G
51	D1	1028	C
51	D1	1030	U
51	D1	1032	G
51	D1	1033	G
51	D1	1034	G
51	D1	1036	A
51	D1	1094	G
51	D1	1099	G
51	D1	1101	A
51	D1	1124	G
51	D1	1130	A
51	D1	1135	U
51	D1	1136	C
51	D1	1137	C
51	D1	1138	G
51	D1	1139	G
51	D1	1158	C
51	D1	1159	U
51	D1	1168	U
51	D1	1182	G
51	D1	1184	G
51	D1	1187	G
51	D1	1191	A
51	D1	1196	A
51	D1	1197	A
51	D1	1200	C
51	D1	1201	A
51	D1	1202	U
51	D1	1207	G
51	D1	1212	U
51	D1	1213	A
51	D1	1225	A
51	D1	1227	A
51	D1	1238	A
51	D1	1241	G
51	D1	1256	A
51	D1	1257	A
51	D1	1258	G
51	D1	1260	G

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Mol	Chain	Res	Type
51	D1	1275	A
51	D1	1278	G
51	D1	1279	G
51	D1	1280	A
51	D1	1281	C
51	D1	1282	C
51	D1	1286	U
51	D1	1287	A
51	D1	1300	G
51	D1	1301	U
51	D1	1305	G
51	D1	1317	C
51	D1	1318	A
51	D1	1320	C
51	D1	1336	C
51	D1	1346	A
51	D1	1347	G
51	D1	1348	U
51	D1	1353	G
51	D1	1363	A
51	D1	1364	U
51	D1	1370	G
51	D1	1379	G
51	D1	1383	C
51	D1	1395	C
51	D1	1396	A
51	D1	1398	A
51	D1	1419	G
51	D1	1446	A
51	D1	1448	C
51	D1	1451	U
51	D1	1452	C
51	D1	1492	A
51	D1	1493	A
51	D1	1494	G
51	D1	1497	G
51	D1	1502	A
51	D1	1503	A
51	D1	1506	U
51	D1	1517	G
51	D1	1529	G
51	D1	1530	G

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Mol	Chain	Res	Type
51	D1	1533	C
51	D1	1534	A
51	D1	1535	C
51	D1	1540	U
52	D2	10	A
52	D2	12	U
52	D2	34	U
52	D2	35	G
52	D2	36	G
52	D2	46	G
52	D2	51	G
52	D2	63	A
52	D2	71	A
52	D2	74	A
52	D2	75	G
52	D2	82	U
52	D2	102	U
52	D2	118	A
52	D2	119	A
52	D2	120	U
52	D2	128	C
52	D2	139	U
52	D2	140	C
52	D2	141	G
52	D2	142	A
52	D2	149	A
52	D2	159	G
52	D2	162	U
52	D2	163	C
52	D2	166	U
52	D2	196	A
52	D2	199	A
52	D2	215	G
52	D2	216	A
52	D2	219	A
52	D2	221	A
52	D2	222	A
52	D2	227	A
52	D2	228	C
52	D2	233	A
52	D2	248	G
52	D2	249	C

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Mol	Chain	Res	Type
52	D2	255	A
52	D2	265	A
52	D2	266	G
52	D2	276	U
52	D2	277	G
52	D2	279	A
52	D2	281	C
52	D2	283	G
52	D2	294	A
52	D2	310	A
52	D2	323	C
52	D2	324	A
52	D2	329	G
52	D2	330	A
52	D2	346	A
52	D2	361	G
52	D2	362	A
52	D2	371	A
52	D2	372	G
52	D2	373	U
52	D2	386	G
52	D2	387	U
52	D2	395	U
52	D2	404	A
52	D2	406	G
52	D2	411	G
52	D2	412	A
52	D2	417	C
52	D2	422	A
52	D2	424	G
52	D2	428	A
52	D2	429	A
52	D2	457	A
52	D2	458	G
52	D2	459	U
52	D2	467	G
52	D2	473	G
52	D2	481	G
52	D2	491	G
52	D2	504	A
52	D2	505	A
52	D2	509	C

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Mol	Chain	Res	Type
52	D2	510	C
52	D2	531	C
52	D2	532	A
52	D2	543	G
52	D2	545	U
52	D2	547	A
52	D2	548	G
52	D2	549	G
52	D2	555	G
52	D2	563	A
52	D2	572	A
52	D2	573	U
52	D2	575	A
52	D2	586	A
52	D2	603	A
52	D2	614	A
52	D2	615	U
52	D2	616	A
52	D2	627	A
52	D2	637	A
52	D2	645	C
52	D2	646	U
52	D2	647	G
52	D2	654	A
52	D2	656	G
52	D2	669	G
52	D2	670	A
52	D2	685	A
52	D2	686	U
52	D2	694	U
52	D2	729	G
52	D2	730	A
52	D2	738	G
52	D2	747	C
52	D2	752	A
52	D2	763	G
52	D2	764	A
52	D2	765	C
52	D2	775	G
52	D2	776	G
52	D2	782	A
52	D2	784	G

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Mol	Chain	Res	Type
52	D2	785	G
52	D2	789	A
52	D2	799	G
52	D2	805	G
52	D2	812	C
52	D2	819	A
52	D2	827	U
52	D2	828	U
52	D2	830	G
52	D2	845	A
52	D2	846	U
52	D2	847	U
52	D2	857	G
52	D2	859	G
52	D2	860	U
52	D2	878	A
52	D2	880	G
52	D2	881	G
52	D2	887	U
52	D2	888	C
52	D2	896	A
52	D2	897	C
52	D2	902	C
52	D2	907	G
52	D2	910	A
52	D2	932	U
52	D2	941	A
52	D2	946	C
52	D2	958	U
52	D2	961	C
52	D2	974	G
52	D2	983	A
52	D2	995	C
52	D2	996	A
52	D2	1005	C
52	D2	1012	U
52	D2	1013	C
52	D2	1021	A
52	D2	1022	G
52	D2	1023	U
52	D2	1024	G
52	D2	1026	G

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Mol	Chain	Res	Type
52	D2	1033	U
52	D2	1046	A
52	D2	1047	G
52	D2	1053	C
52	D2	1057	A
52	D2	1058	U
52	D2	1060	U
52	D2	1061	U
52	D2	1062	G
52	D2	1066	U
52	D2	1068	G
52	D2	1069	A
52	D2	1070	A
52	D2	1071	G
52	D2	1074	G
52	D2	1075	C
52	D2	1076	C
52	D2	1080	A
52	D2	1081	U
52	D2	1082	U
52	D2	1083	U
52	D2	1084	A
52	D2	1085	A
52	D2	1087	G
52	D2	1088	A
52	D2	1090	A
52	D2	1103	A
52	D2	1104	C
52	D2	1111	A
52	D2	1130	U
52	D2	1131	G
52	D2	1132	U
52	D2	1135	C
52	D2	1139	G
52	D2	1171	G
52	D2	1172	C
52	D2	1175	A
52	D2	1176	U
52	D2	1177	G
52	D2	1178	C
52	D2	1179	G
52	D2	1180	U

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Mol	Chain	Res	Type
52	D2	1206	G
52	D2	1211	C
52	D2	1212	G
52	D2	1237	A
52	D2	1250	G
52	D2	1251	C
52	D2	1253	A
52	D2	1256	G
52	D2	1271	G
52	D2	1272	A
52	D2	1273	U
52	D2	1300	G
52	D2	1301	A
52	D2	1306	C
52	D2	1329	U
52	D2	1330	C
52	D2	1345	C
52	D2	1352	U
52	D2	1359	A
52	D2	1365	A
52	D2	1368	G
52	D2	1378	A
52	D2	1379	U
52	D2	1383	A
52	D2	1395	A
52	D2	1397	U
52	D2	1416	G
52	D2	1417	C
52	D2	1419	A
52	D2	1420	A
52	D2	1421	G
52	D2	1427	A
52	D2	1428	C
52	D2	1437	C
52	D2	1452	G
52	D2	1453	A
52	D2	1454	C
52	D2	1458	U
52	D2	1459	G
52	D2	1461	C
52	D2	1475	G
52	D2	1482	G

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Mol	Chain	Res	Type
52	D2	1483	G
52	D2	1490	A
52	D2	1491	G
52	D2	1504	A
52	D2	1508	A
52	D2	1515	A
52	D2	1519	G
52	D2	1524	G
52	D2	1532	A
52	D2	1535	A
52	D2	1536	C
52	D2	1537	G
52	D2	1555	G
52	D2	1558	C
52	D2	1560	G
52	D2	1565	C
52	D2	1569	A
52	D2	1578	U
52	D2	1581	G
52	D2	1583	A
52	D2	1585	C
52	D2	1608	A
52	D2	1610	A
52	D2	1611	C
52	D2	1616	A
52	D2	1647	U
52	D2	1648	U
52	D2	1654	A
52	D2	1674	G
52	D2	1715	G
52	D2	1730	C
52	D2	1731	G
52	D2	1738	G
52	D2	1758	U
52	D2	1764	C
52	D2	1773	A
52	D2	1776	G
52	D2	1784	A
52	D2	1791	A
52	D2	1800	C
52	D2	1801	A
52	D2	1802	A

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Mol	Chain	Res	Type
52	D2	1808	A
52	D2	1812	U
52	D2	1816	C
52	D2	1828	G
52	D2	1829	A
52	D2	1842	G
52	D2	1847	A
52	D2	1857	G
52	D2	1859	U
52	D2	1870	C
52	D2	1871	A
52	D2	1884	G
52	D2	1901	A
52	D2	1905	C
52	D2	1906	G
52	D2	1914	C
52	D2	1929	G
52	D2	1930	G
52	D2	1931	U
52	D2	1937	A
52	D2	1938	A
52	D2	1941	C
52	D2	1955	U
52	D2	1966	A
52	D2	1967	C
52	D2	1970	A
52	D2	1971	U
52	D2	1972	G
52	D2	1991	U
52	D2	1993	U
52	D2	1997	C
52	D2	2022	U
52	D2	2023	C
52	D2	2027	G
52	D2	2031	A
52	D2	2033	A
52	D2	2043	C
52	D2	2052	A
52	D2	2055	C
52	D2	2056	G
52	D2	2060	A
52	D2	2061	G

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Mol	Chain	Res	Type
52	D2	2062	A
52	D2	2069	G
52	D2	2093	G
52	D2	2096	C
52	D2	2102	G
52	D2	2110	G
52	D2	2111	U
52	D2	2112	G
52	D2	2114	A
52	D2	2117	A
52	D2	2118	U
52	D2	2119	A
52	D2	2130	U
52	D2	2131	U
52	D2	2132	U
52	D2	2133	G
52	D2	2136	G
52	D2	2140	G
52	D2	2145	C
52	D2	2146	C
52	D2	2147	A
52	D2	2149	U
52	D2	2156	G
52	D2	2159	G
52	D2	2160	C
52	D2	2162	G
52	D2	2166	U
52	D2	2168	G
52	D2	2169	A
52	D2	2170	A
52	D2	2171	A
52	D2	2172	U
52	D2	2173	A
52	D2	2174	C
52	D2	2178	C
52	D2	2183	A
52	D2	2186	G
52	D2	2189	U
52	D2	2192	U
52	D2	2198	A
52	D2	2199	A
52	D2	2203	U

Continued on next page...

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Mol	Chain	Res	Type
52	D2	2204	G
52	D2	2211	A
52	D2	2213	U
52	D2	2225	A
52	D2	2226	C
52	D2	2238	G
52	D2	2239	G
52	D2	2250	G
52	D2	2278	A
52	D2	2283	C
52	D2	2286	G
52	D2	2287	A
52	D2	2297	A
52	D2	2305	U
52	D2	2308	G
52	D2	2309	A
52	D2	2320	U
52	D2	2325	G
52	D2	2327	A
52	D2	2334	U
52	D2	2345	G
52	D2	2350	C
52	D2	2361	G
52	D2	2383	G
52	D2	2385	C
52	D2	2389	G
52	D2	2392	A
52	D2	2402	U
52	D2	2403	C
52	D2	2406	A
52	D2	2423	U
52	D2	2424	C
52	D2	2425	A
52	D2	2429	G
52	D2	2430	A
52	D2	2441	U
52	D2	2447	G
52	D2	2448	A
52	D2	2459	A
52	D2	2476	A
52	D2	2478	A
52	D2	2491	U

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Mol	Chain	Res	Type
52	D2	2494	G
52	D2	2497	A
52	D2	2502	G
52	D2	2503	A
52	D2	2505	G
52	D2	2518	A
52	D2	2520	C
52	D2	2529	G
52	D2	2535	G
52	D2	2547	A
52	D2	2554	U
52	D2	2566	A
52	D2	2567	G
52	D2	2572	A
52	D2	2573	C
52	D2	2602	A
52	D2	2603	G
52	D2	2609	U
52	D2	2613	U
52	D2	2615	U
52	D2	2629	U
52	D2	2630	G
52	D2	2646	C
52	D2	2655	G
52	D2	2656	U
52	D2	2682	A
52	D2	2689	U
52	D2	2690	U
52	D2	2714	G
52	D2	2722	G
52	D2	2724	U
52	D2	2732	G
52	D2	2733	A
52	D2	2744	G
52	D2	2748	A
52	D2	2764	A
52	D2	2765	A
52	D2	2778	A
52	D2	2779	U
52	D2	2780	G
52	D2	2791	G
52	D2	2797	U

Continued on next page...

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Mol	Chain	Res	Type
52	D2	2798	U
52	D2	2799	A
52	D2	2800	A
52	D2	2808	G
52	D2	2820	A
52	D2	2823	A
52	D2	2833	U
52	D2	2834	G
52	D2	2848	G
52	D2	2849	U
52	D2	2867	G
52	D2	2868	A
52	D2	2872	A
52	D2	2873	A
52	D2	2880	C
52	D2	2884	U
52	D2	2887	A
52	D2	2901	C
52	D2	2902	C
52	D2	2903	U
53	D3	4	C
53	D3	9	G
53	D3	12	C
53	D3	13	G
53	D3	23	G
53	D3	26	C
53	D3	35	C
53	D3	41	G
53	D3	44	G
53	D3	66	A
53	D3	67	G
53	D3	87	U
53	D3	88	C
53	D3	89	U
53	D3	90	C
53	D3	108	A
53	D3	109	A
53	D3	116	G
53	D3	120	A
54	D4	13	A
55	D5	9	G
55	D5	17	C

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Mol	Chain	Res	Type
55	D5	19	G
55	D5	20	U
55	D5	47	U
55	D5	48	C
55	D5	49	G
55	D5	74	C
55	D5	76	A

All (35) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
51	D1	70	U
51	D1	686	U
51	D1	871	U
51	D1	890	G
51	D1	1190	G
51	D1	1196	A
51	D1	1201	A
51	D1	1300	G
51	D1	1347	G
52	D2	227	A
52	D2	328	U
52	D2	372	G
52	D2	421	C
52	D2	458	G
52	D2	490	C
52	D2	615	U
52	D2	774	G
52	D2	784	G
52	D2	858	G
52	D2	859	G
52	D2	1020	A
52	D2	1236	G
52	D2	1328	A
52	D2	1358	G
52	D2	1490	A
52	D2	1730	C
52	D2	1900	A
52	D2	1930	G
52	D2	2333	A
52	D2	2391	G
52	D2	2423	U

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Mol	Chain	Res	Type
52	D2	2629	U
52	D2	2655	G
52	D2	2832	U
53	D3	88	C

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
55	FME	D5	77	55	8,9,10	0.38	0	7,9,11	1.15	1 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	FME	D5	77	55	-	3/7/9/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	D5	77	FME	CA-N-CN	2.41	126.53	122.82

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	D5	77	FME	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
55	D5	77	FME	C-CA-CB-CG
55	D5	77	FME	CB-CG-SD-CE

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

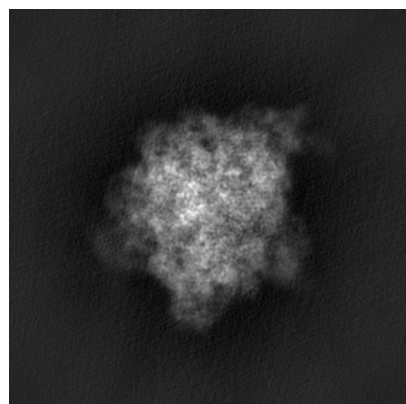
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-56038. These allow visual inspection of the internal detail of the map and identification of artifacts.

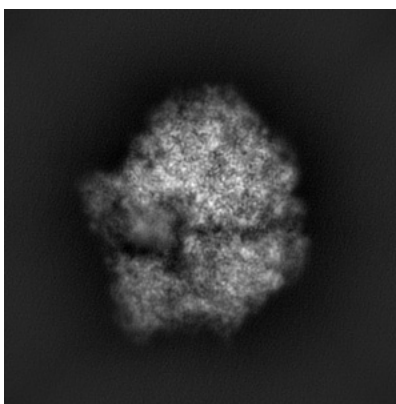
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

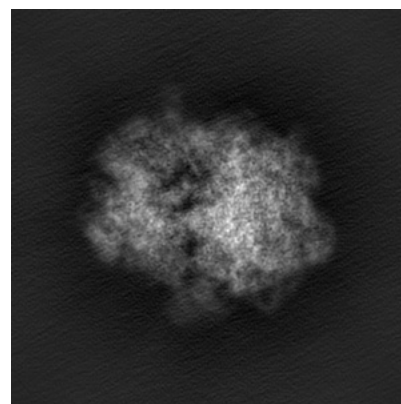
6.1.1 Primary map



X

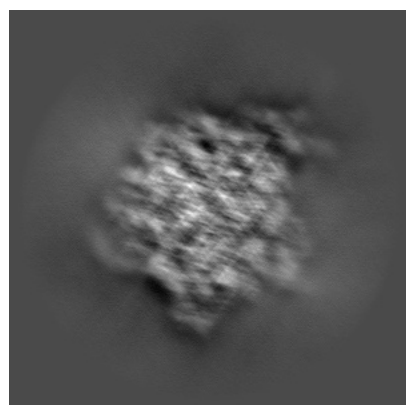


Y

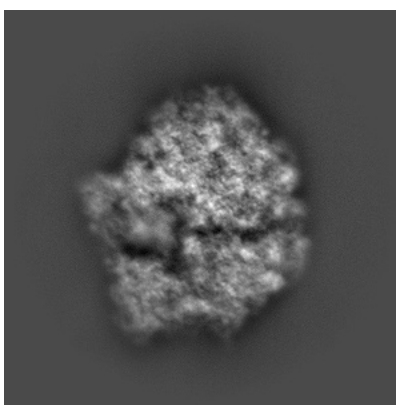


Z

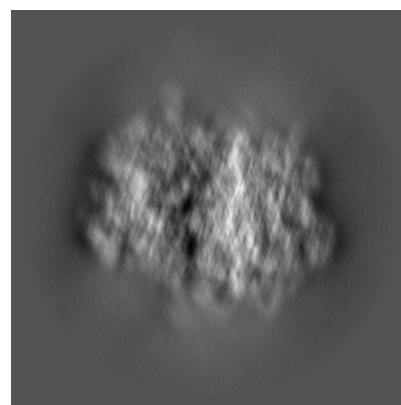
6.1.2 Raw map



X



Y

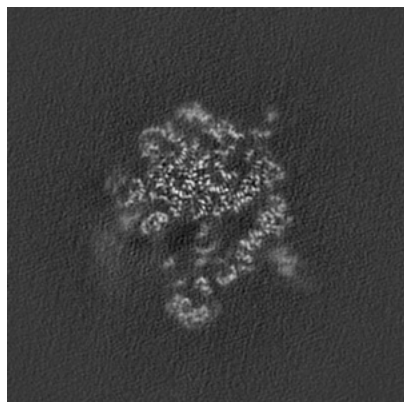


Z

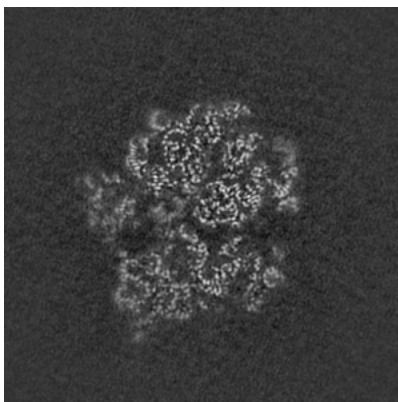
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

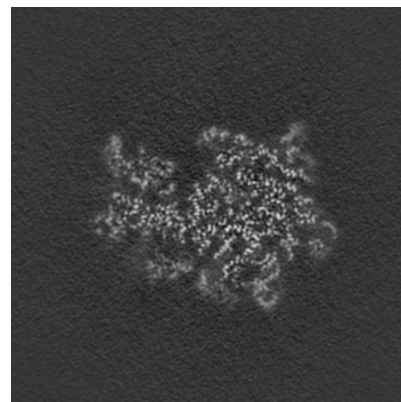
6.2.1 Primary map



X Index: 240

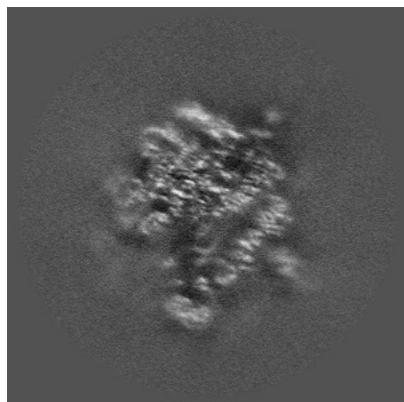


Y Index: 240

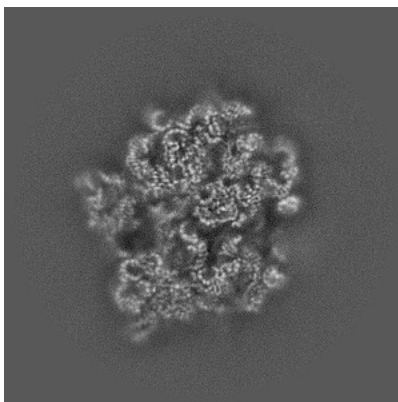


Z Index: 240

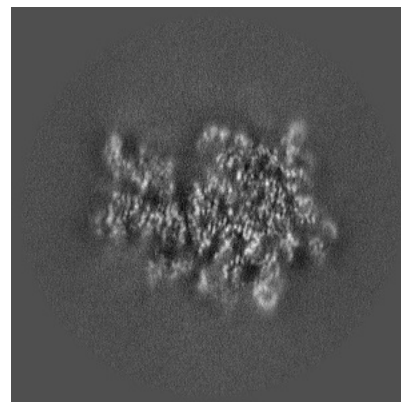
6.2.2 Raw map



X Index: 240



Y Index: 240

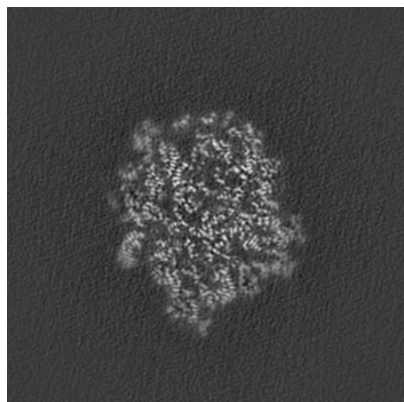


Z Index: 240

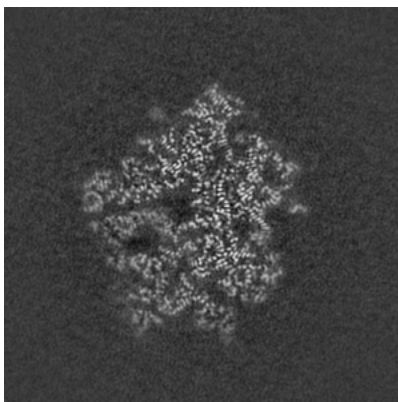
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

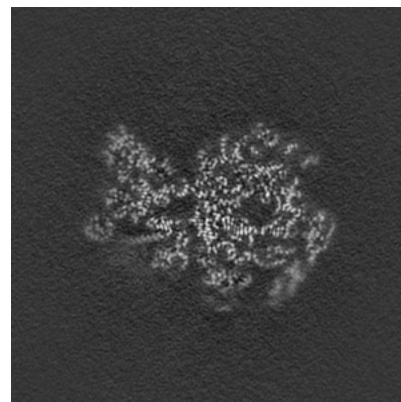
6.3.1 Primary map



X Index: 270

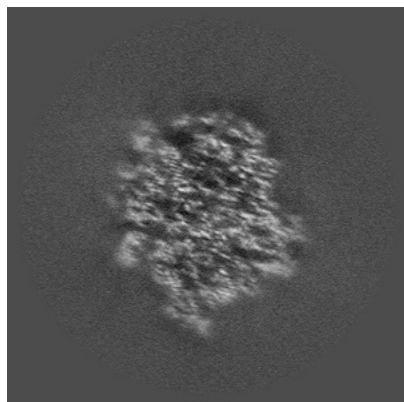


Y Index: 223

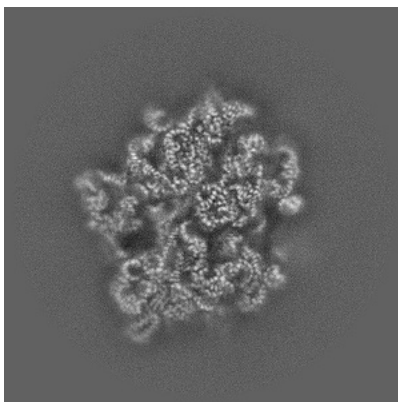


Z Index: 257

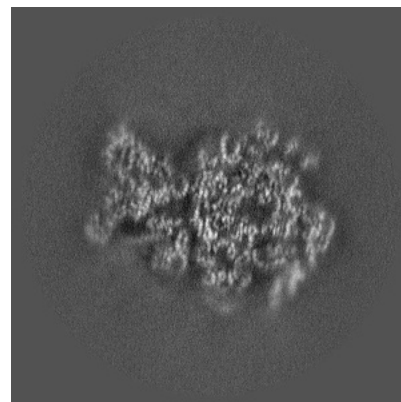
6.3.2 Raw map



X Index: 269



Y Index: 236

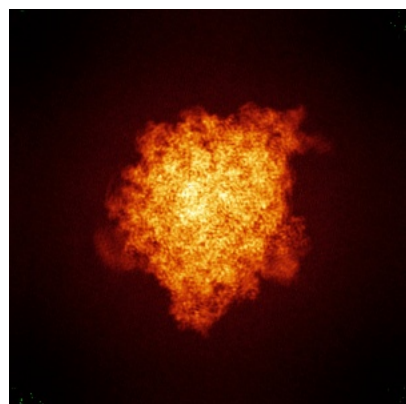


Z Index: 256

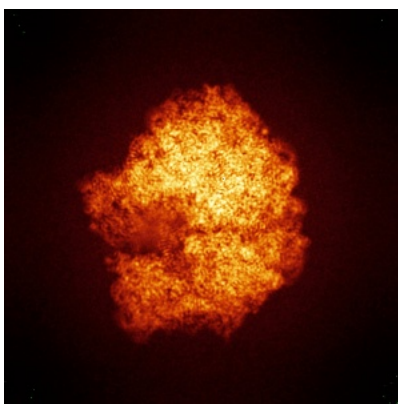
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

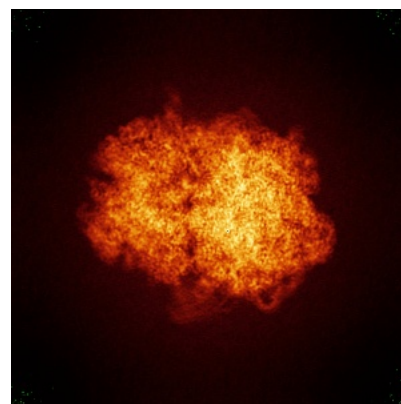
6.4.1 Primary map



X

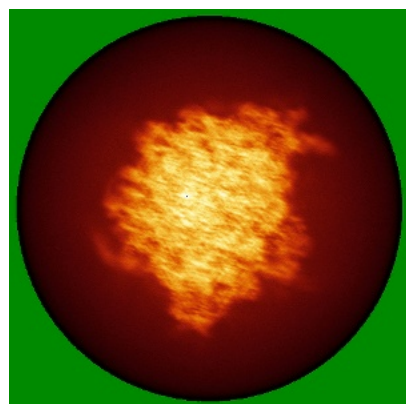


Y

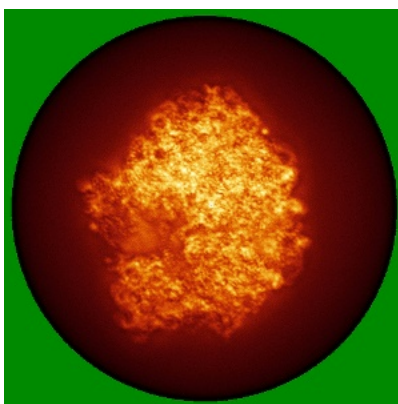


Z

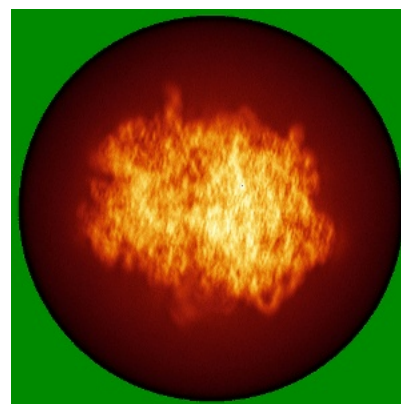
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

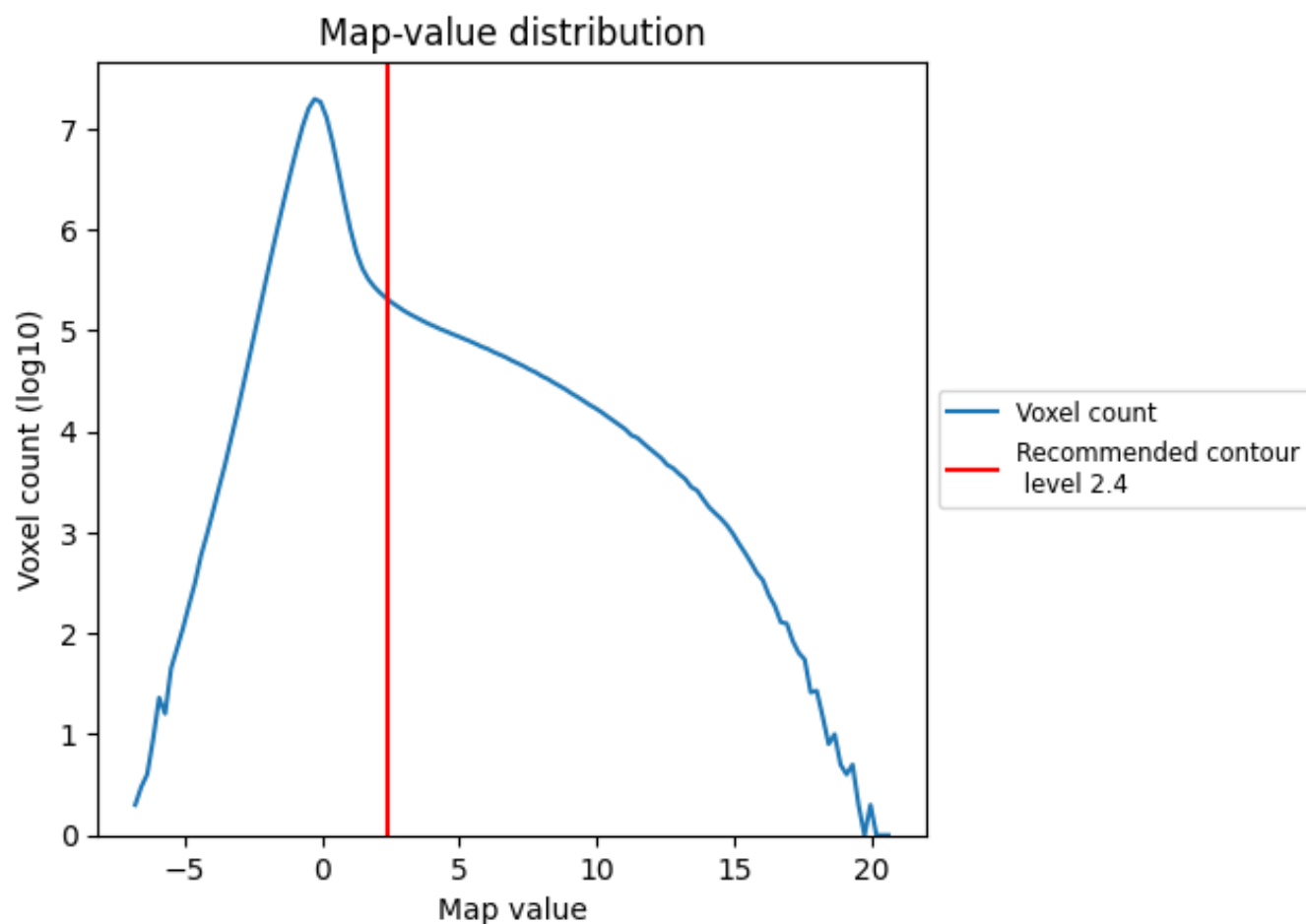
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

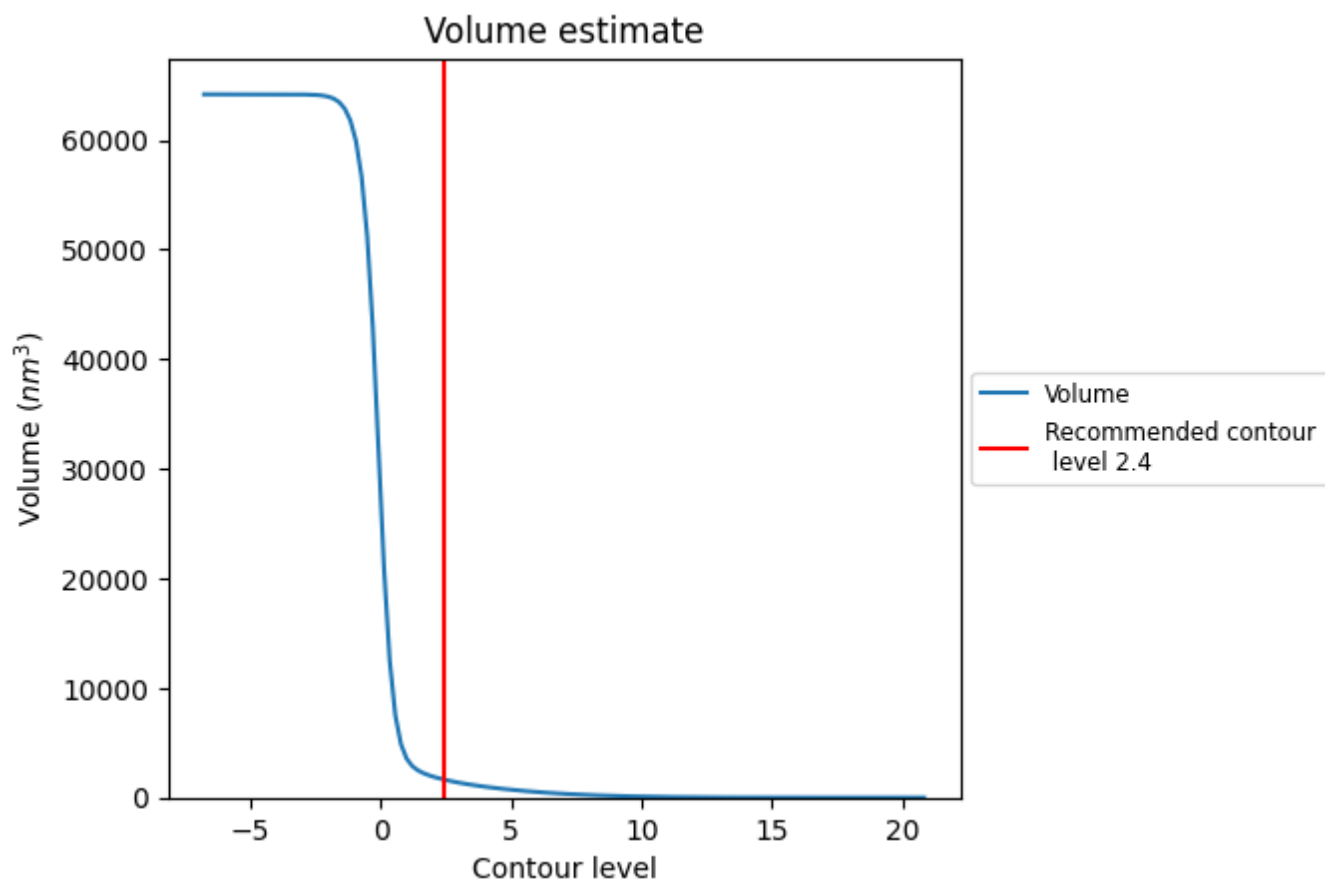
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

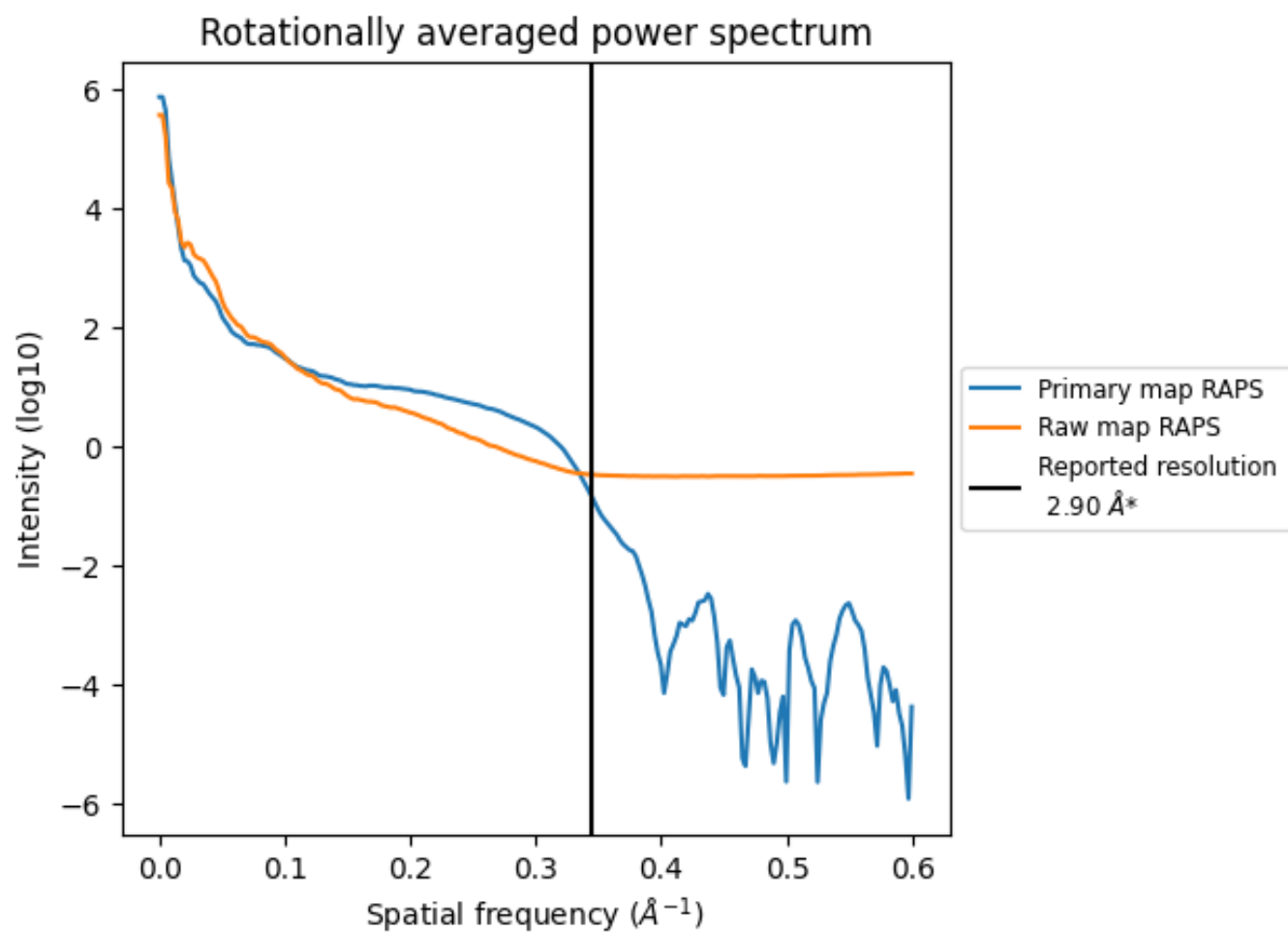
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1650 nm^3 ; this corresponds to an approximate mass of 1490 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

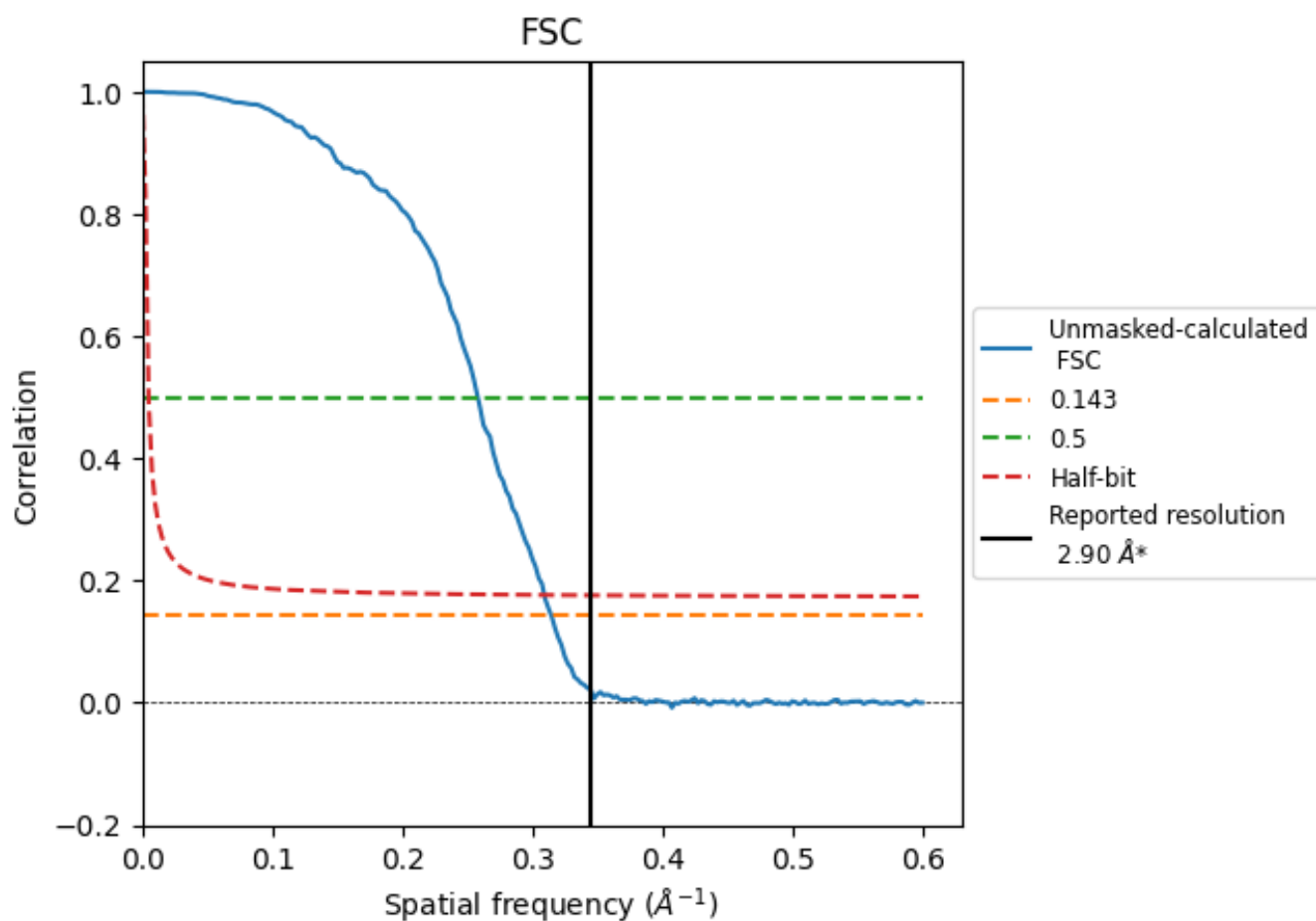


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8.2 Resolution estimates [i](#)

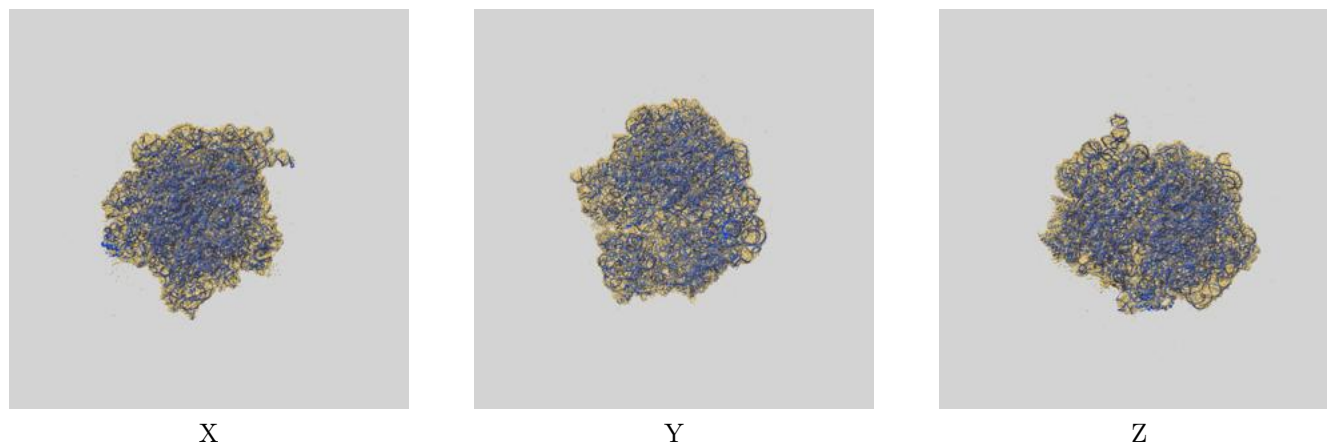
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.18	3.88	3.24

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

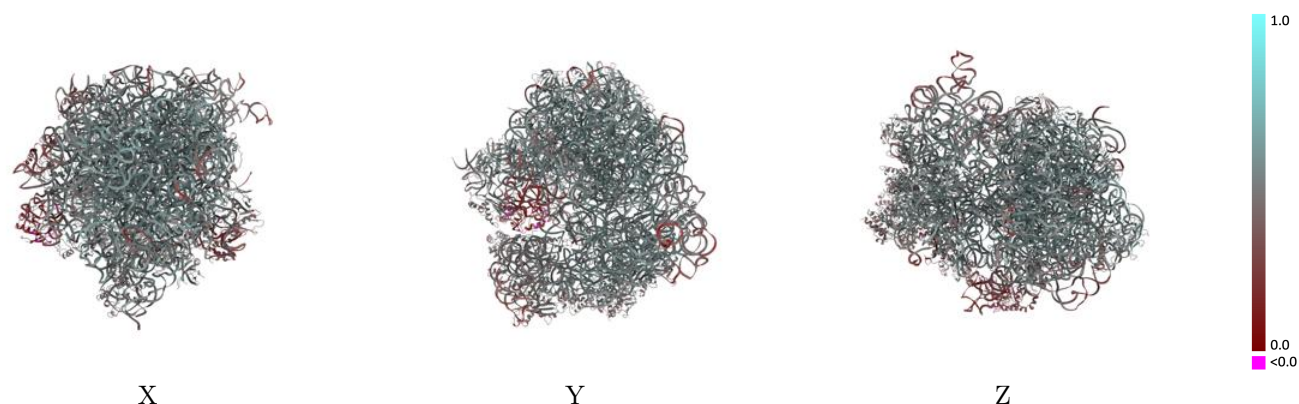
This section contains information regarding the fit between EMDB map EMD-56038 and PDB model 9TKR. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



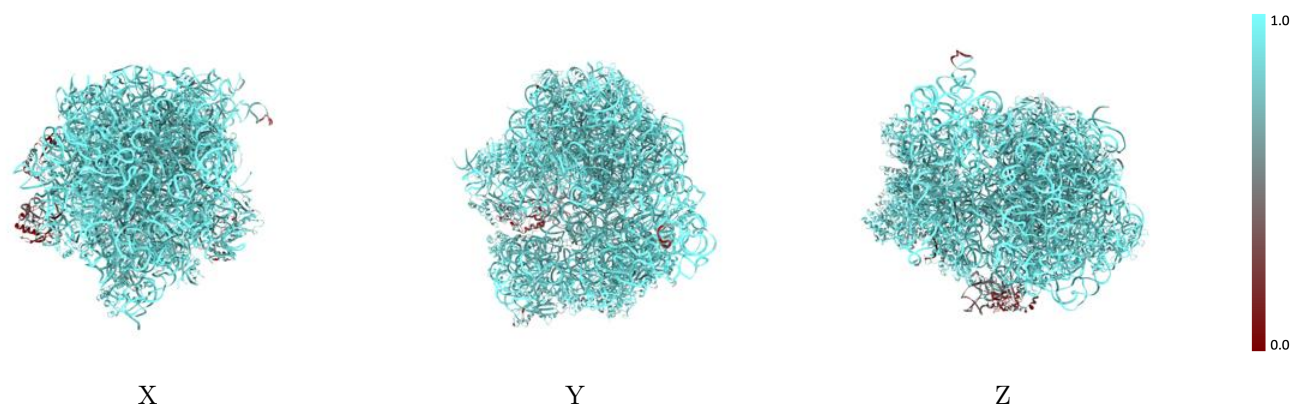
The images above show the 3D surface view of the map at the recommended contour level 2.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



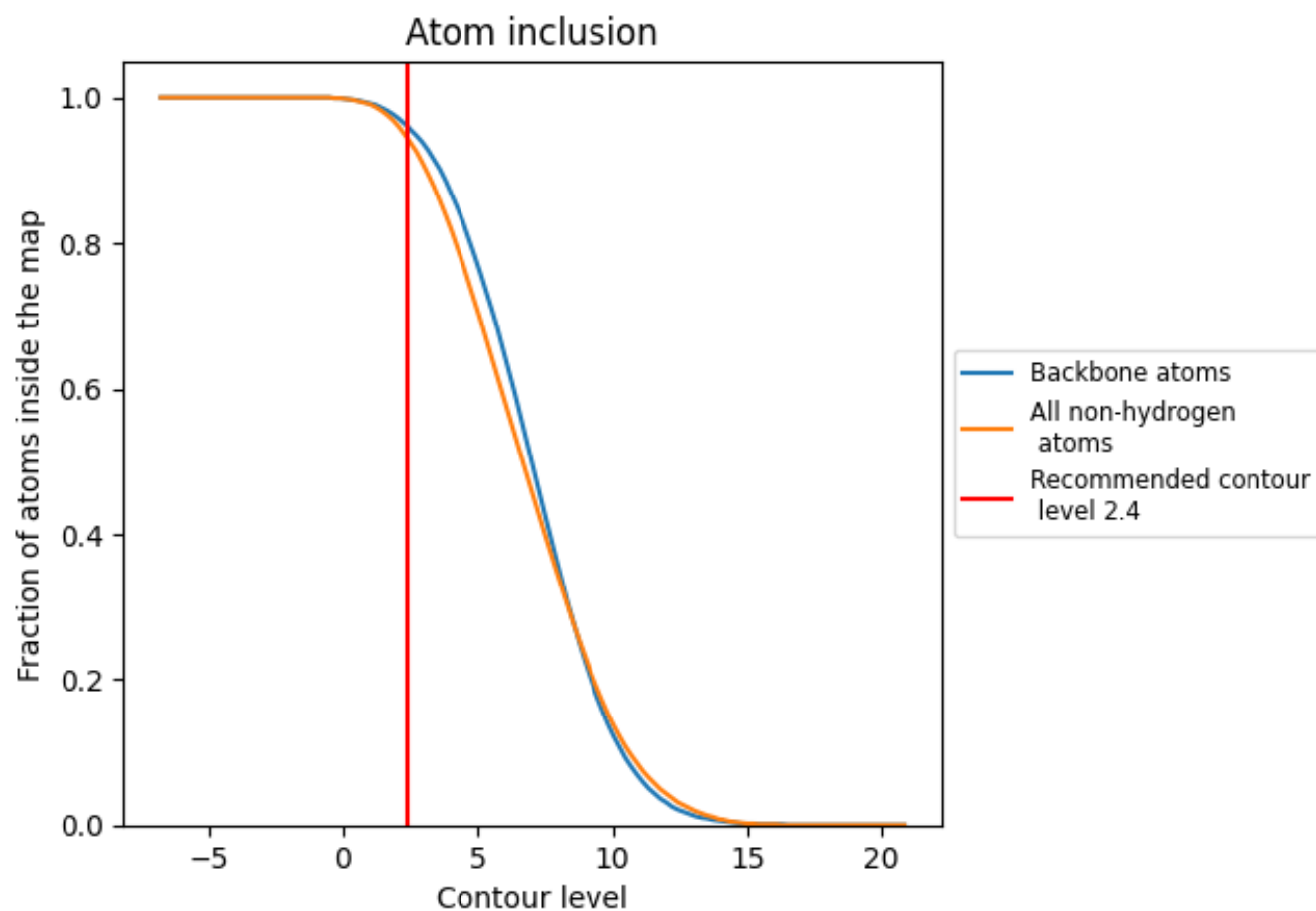
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (2.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9430	 0.4930
AA	 0.8500	 0.4390
AB	 0.9020	 0.4780
AC	 0.8940	 0.4670
AD	 0.9280	 0.4970
AE	 0.9160	 0.4390
AF	 0.8780	 0.4200
AG	 0.9300	 0.5030
AH	 0.8940	 0.4310
AI	 0.8040	 0.4120
AJ	 0.9440	 0.4850
AK	 0.9230	 0.5140
AL	 0.8730	 0.4450
AM	 0.8880	 0.4500
AN	 0.9230	 0.4720
AO	 0.9010	 0.4870
AP	 0.9150	 0.4830
AQ	 0.9220	 0.4610
AR	 0.8420	 0.4380
AS	 0.9170	 0.4760
AT	 0.7270	 0.3340
B0	 0.9410	 0.5490
B1	 0.9550	 0.5230
B2	 0.8910	 0.4300
B3	 0.9380	 0.5140
B5	 0.9460	 0.5220
B6	 0.9300	 0.4810
B7	 0.9800	 0.5500
B8	 0.9630	 0.5620
B9	 0.9660	 0.5260
BA	 0.1180	 0.2050
BB	 0.9590	 0.5430
BC	 0.9520	 0.5290
BD	 0.9150	 0.5030
BE	 0.8870	 0.4390



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Chain	Atom inclusion	Q-score
BF	 0.8600	 0.4340
BI	 0.4210	 0.3300
BK	 0.4030	 0.2340
BM	 0.9560	 0.5260
BN	 0.9430	 0.5280
BO	 0.9440	 0.5120
BP	 0.9660	 0.5270
BQ	 0.9680	 0.5340
BR	 0.9260	 0.4710
BS	 0.9460	 0.5310
BT	 0.9640	 0.5400
BU	 0.9220	 0.5130
BV	 0.9440	 0.5350
BW	 0.9350	 0.5060
BX	 0.9280	 0.4970
BY	 0.9320	 0.4960
D1	 0.9780	 0.4970
D2	 0.9740	 0.5090
D3	 0.9890	 0.4980
D4	 0.7190	 0.3800
D5	 0.9340	 0.4590